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SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's full Name: Devsh Khare Examiner #: 77931 Date: 3/27/2003
 Art Unit: 1623 Phone Number 605-1199 Serial Number: 09/828,276
 Mail Box: CM1-8B19 and Bldg/Room Location: CM1-8A13 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be search Include the elected species or structures, key words, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: See Bib Data Sheet

Inventors (please provide full names): See Bib Data Sheet

Earliest priority Filing Date: See Bib Data Sheet

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please carry out a structure search for the compounds in claims 1 and 10 (claims 1-16) and their pharmaceutical compositions. A copy of the claims is provided.

The Bib Data Sheet which discloses the inventor names, title of the invention, and the earliest priority filing date is also provided.

Note: Please return the copy of the claims with the search.

Thank you.

POINT OF CONTACT:
 PAUL SCHULWITZ
 TECHNICAL INFO. SPECIALIST
 CM1 6B06 TEL. (703) 305-1954

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	Type of Search	Vendors and cost where applicable
Searcher: _____	NA Sequence (#) _____	STN <u>1241.40</u>
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>8</u>	Questel/Orbit _____
Date Searcher Picked Up: <u>3/28</u>	Bibliographic _____	Dr. Link _____
Date Completed: <u>4/3</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>8:60</u>	Fulltext _____	Sequence Systems _____
Clerical prep time: _____	Patent Family _____	WWW/Internet _____
Online Time: <u>82</u>	Other _____	Other (specify) _____

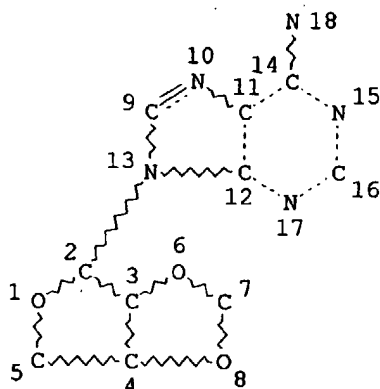
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NODE ATTRIBUTES:

NSPEC IS RC AT 18
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

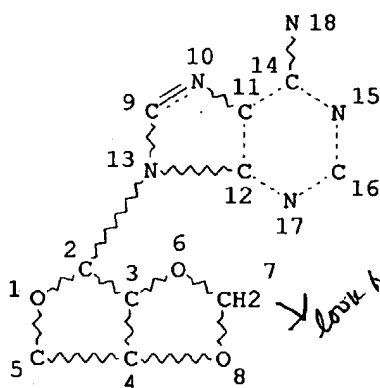
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L2 3214 SEA FILE=REGISTRY SSS FUL L1

L3 STR



NODE ATTRIBUTES:

NSPEC IS RC AT 18
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L4 15 SEA FILE=REGISTRY SUB=L2 SSS FUL L3
L30 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L4

=> d ibib abs hitstr l30 1-10

L30 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1993:204739 HCAPLUS

DOCUMENT NUMBER: 118:204739

TITLE: 2',3'-O-Cyclic derivatives of ribonucleosides and
their 5'-phosphonates: synthesis and anti-HIV
activity

AUTHOR(S): Atrazheva, E. D.; Lukin, M. A.; Yasko, M. V.;
Shushkov, T. V.; Tarussova, N. B.; Kraevskii, A.;
Balzarini, Jan; De Clercq, Erik

CORPORATE SOURCE: V. A. Engel'khardt Inst. Mol. Biol., Moscow, 117984,
Russia

SOURCE: Medicinal Chemistry Research (1991), 1(2), 155-65
CODEN: MCREEB; ISSN: 1054-2523

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Several 2',3'-O-orthoesters, 2',3'-O-ketals and 2',3'-O-acetals of
ribonucleosides and their 5'-phosphonates were synthesized. In some cases
urine diastereomers were either isolated from the racemate mixts. or
stereospecifically synthesized. Some nucleosides and their
5'-phosphonates were effective in suppressing HIV-1 replication in MT-4
cells. Of the nucleosides, 2',3'-O-methoxymethyleneguanosine (both R and
S diastereomers) and 2',3'-O-methoxymethylenecytidine showed some anti-HIV
activity. However, a more pronounced anti-HIV activity, with selectivity
indexes of 2-3 orders of magnitude, was exhibited by the
5'-hydrogenphosphonates of 2',3'-O-methoxymethyleneadenosine (R
diastereomer), 2',3'-O-methoxymethylenecytidine, 2',3'-O-
methoxymethyleneguanosine as well as 2',3'-O-ethoxymethyleneadenosine
5'-hydroxymethylphosphonate (R diastereomer).

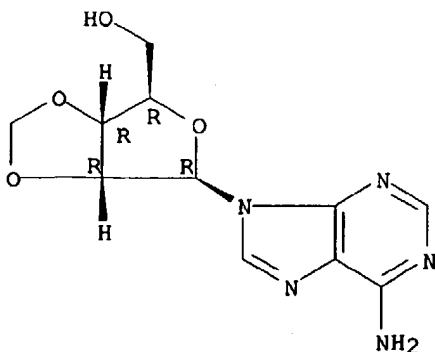
IT 4137-31-9P 143992-71-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and human immunodeficiency virus inhibition by)

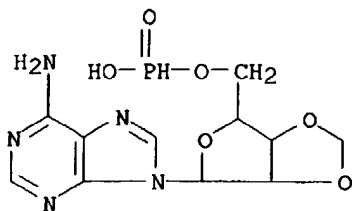
RN 4137-31-9 HCAPLUS

CN Adenosine, 2',3'-O-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

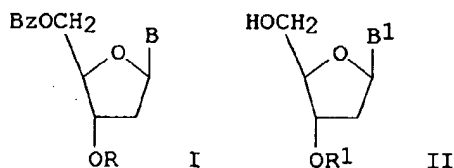
Absolute stereochemistry.



RN 143992-71-6 HCAPLUS
 CN Adenosine, 2',3'-O-methylene-, 5'-(hydrogen phosphonate) (9CI) (CA INDEX NAME)



L30 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1992:427016 HCAPLUS
 DOCUMENT NUMBER: 117:27016
 TITLE: 1-Alkylthioalkylation of nucleoside hydroxyl functions and its synthetic applications: a new versatile method in nucleoside chemistry
 AUTHOR(S): Zavgorodnii, S.; Polyanskii, M.; Besidskii, E.; Kryukov, V.; Sanin, A.; Pokrovakaya, M.; Gurskaya, G.; Lonnberg, Harri; Azhaev, A.
 CORPORATE SOURCE: Chimtech Ltd., Moscow, 117871, USSR
 SOURCE: Tetrahedron Letters (1991), 32(51), 7593-6
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

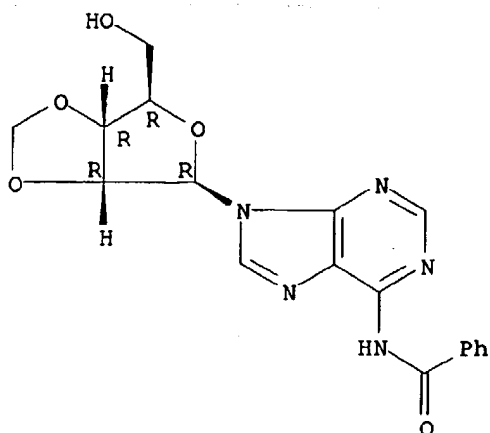


AB Treatment of appropriately protected nucleosides I (B = Thy, BzCyt, BzAde, IbGua; R = H) with a mixt. of acetic acid, acetic anhydride and dialkyl sulfoxide was shown to give O-(1-alkylthioalkylated) nucleosides I (R = CH₂SMe) that were oxidized to the corresponding sulfoxides and sulfones I (R = CH₂S(O)nMe, n = 1, 2), or converted via O-halomethyl derivs. I (R = CH₂Br, CH₂Cl) to various O-substituted nucleosides, e.g., II, [B1 = Thy, Cyt, Ade, Gua; R1 = CH₂F, CH₂N₃, CH₂CN, CH₂OMe, CH₂P(O)(OH)₂].

IT 139434-75-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 139434-75-6 HCAPLUS
 CN Adenosine, N-benzoyl-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L30 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1990:441207 HCAPLUS

DOCUMENT NUMBER: 113:41207

TITLE: Synthesis of the 2-chloro analogs of 3'-deoxyadenosine, 2',3'-dideoxyadenosine, and 2',3'-didehydro-2',3'-dideoxyadenosine as potential antiviral agents [Erratum to document cited in CA110(21):193310x]

AUTHOR(S): Rosowsky, Andre; Solan, Vishnu C.; Sodroski, Joseph G.; Ruprecht, Ruth M.

CORPORATE SOURCE: Dana-Farber Cancer Inst., Harvard Med. Sch., Boston, MA, 02115, USA

SOURCE: Journal of Medicinal Chemistry (1990), 33(4), 1270
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Errors in the text have been cor. The errors were not reflected in the abstr. or the index entries.

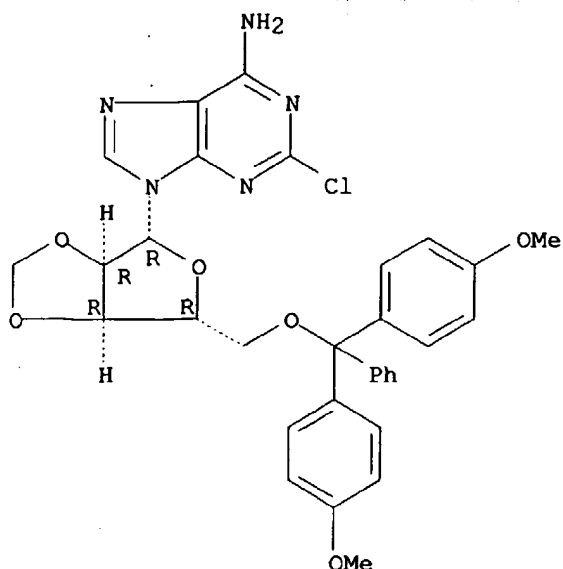
IT 119530-61-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and detritylation of (Erratum))

RN 119530-61-9 HCAPLUS

CN Adenosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2-chloro-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



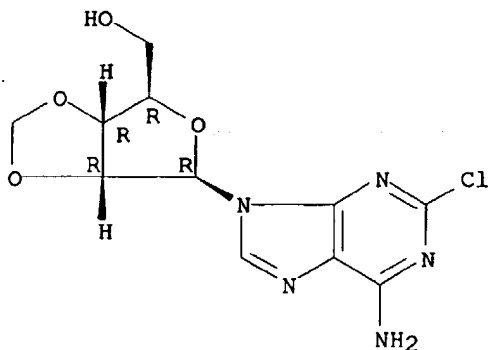
IT 119530-63-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of (Erratum))

RN 119530-63-1 HCAPLUS

CN Adenosine, 2-chloro-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L30 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2003 ACS

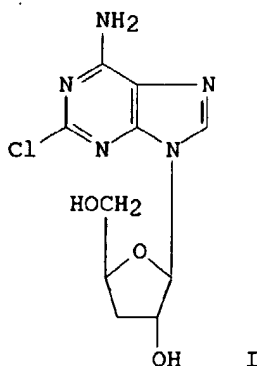
ACCESSION NUMBER: 1989:193310 HCAPLUS

DOCUMENT NUMBER: 110:193310

TITLE: Synthesis of the 2-chloro analogs of
3'-deoxyadenosine, 2',3'-dideoxyadenosine, and
2',3'-didehydro-2',3'-dideoxyadenosine as potential
antiviral agentsAUTHOR(S): Rosowsky, Andre; Solan, Vishnu C.; Sodroski, Joseph
G.; Ruprecht, Ruth M.

CORPORATE SOURCE: Dana-Farber Cancer Inst., Harvard Med. Sch., Boston,

SOURCE: MA, 02115, USA
Journal of Medicinal Chemistry (1989), 32(5), 1135-40
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:193310
GI



AB 2-Chloro-3'-deoxyadenosine (I), 2-chloro-2',3'-dideoxyadenosine (II), and 2-chloro-2',3'-dideoxyadenosine (III) were synthesized from 2-chloroadenosine as candidate antiretroviral agents on the basis that 2-chloro substitution would prevent enzymic deamination and increase efficacy relative to 2',3'-dideoxyadenosine. Redn. of 2-chloro-5'-O-(4,4'-dimethoxytrityl)-2',3'-O-thiocarbonyl-adenosine (IV) with Bu₃SnH, followed by detritylation with AcOH, unexpectedly gave a mixt. of I and 2-chloroadenine. Treatment of the crude Bu₃SnH redn. product with 1,1'-thiocarbonyldiimidazole, followed by another cycle of Bu₃SnH redn. and detritylation with silica gel afforded II and a byproduct identified as 2-chloro-2',3'-O-methyleneadenosine. Treatment of IV with 1,3-dimethyl-2-phenyl-1,3,2-diazaphospholidine followed by silica gel detritylation afforded III. II and III were tested for activity against human immunodeficiency virus (HIV) in a cultured human T4+ lymphocyte cell line. At a concn. of 100 .mu.M, II inhibited reverse transcriptase (RT) prodn. by 97%, while 2',3'-dideoxyadenosine (V) gave >99% inhibition. In growth assays against uninfected T4+ cells, however, 100 .mu.M II gave 23% inhibition while 100 .mu.M V was nontoxic. At a nontoxic concn. of 20 .mu.M, RT prodn. was 75% inhibited by V but only 43% inhibited by II. Thus, a 2-chloro substituent increased host cell toxicity but decreased antiretroviral activity. III was more cytotoxic than II, and antiviral effects could not be measured above 20 .mu.M, where there was only 75% inhibition of RT prodn. Because of the decreased therapeutic index of III relative to II and V, >90% inhibition of viral protein synthesis at a noncytotoxic concn. could not be achieved. In growth assays with cultured human T and B lymphocytes, 100 .mu.M I gave 60-70% growth inhibition, while the IC₅₀ against mouse fibroblasts was only 30 .mu.M. The high cytotoxicity of I precluded consideration of this compd. as an antiviral agent.

IT 119530-61-9P

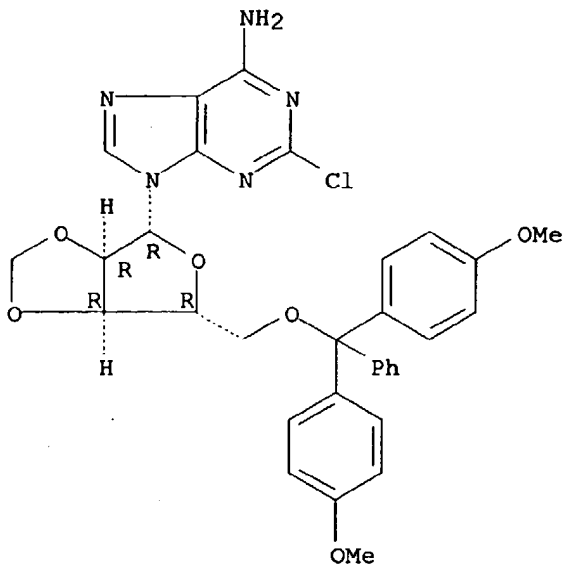
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and detritylation of)

RN 119530-61-9 HCAPLUS

CN Adenosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2-chloro-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



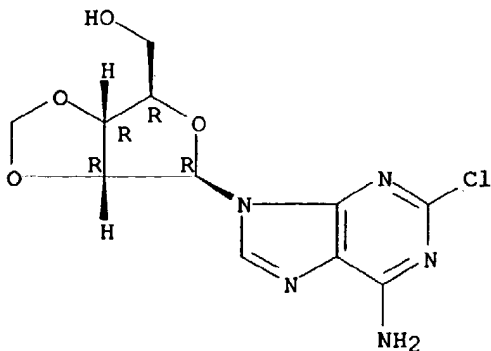
IT 119530-63-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 119530-63-1 HCAPLUS

CN Adenosine, 2-chloro-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L30 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1987:472985 HCAPLUS

DOCUMENT NUMBER: 107:72985

TITLE: A proton magnetic resonance study of the effects of polyamine and divalent metal ions on diadenosine 5', 5'''-P1,P4-tetraphosphate base stacking

AUTHOR(S): Westkaemper, Richard B.

CORPORATE SOURCE: Sch. Pharm., Virginia Commonwealth Univ., Richmond, VA, 23298, USA

SOURCE: Biochemical and Biophysical Research Communications (1987), 144(2), 922-9
CODEN: BBRCA9; ISSN: 0006-291X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complexation of putrescine, spermidine, spermine, and Mg²⁺ with diadenosine 5', 5'''-P1, P4-tetraphosphate induces an upfield shift in the NMR signals for the H-2 and H-8 protons. The upfield shifts in H-2 indicate that cation complexation enhances intramol. adenine stacking interactions. The resonances for H-2 and H-8 of neutral analogs of 5',5'-dinucleotides appear farther upfield relative to the appropriate monomeric models than those for the corresponding dinucleotide; redn. of intra-chain phosphate repulsion is the origin of cation induced enhancement of diadenosine 5',5'''-P1,P4-tetraphosphate base stacking.

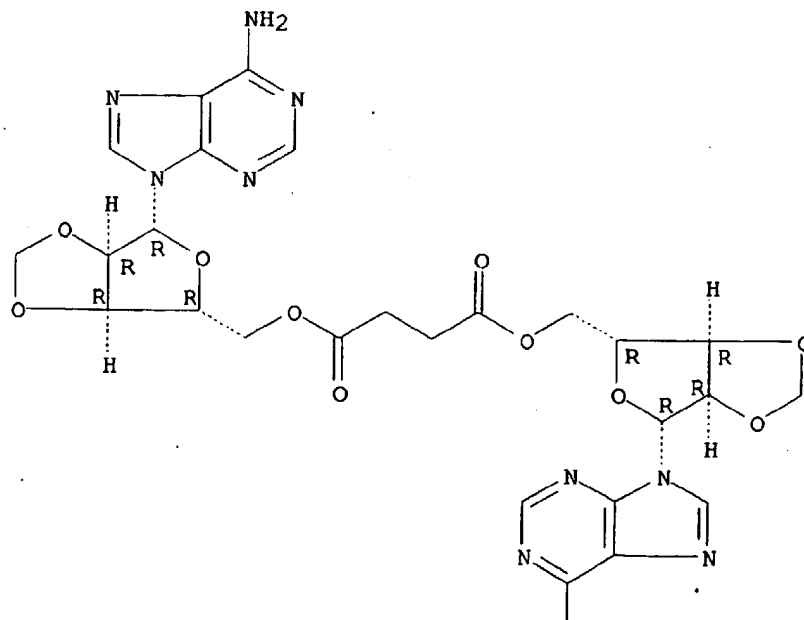
IT 109828-20-8P 109828-21-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

RN 109828-20-8 HCAPLUS

CN Adenosine, 2',3'-O-methylene-, 5',5'''-butanedioate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

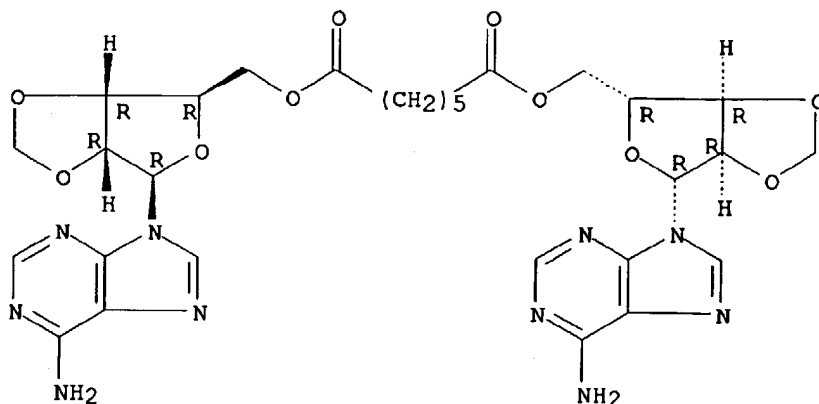


PAGE 2-A



RN 109828-21-9 HCAPLUS
 CN Adenosine, 2',3'-O-methylene-, 5',5'''-heptanedioate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L30 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1986:551228 HCAPLUS

DOCUMENT NUMBER: 105:151228

TITLE: Biological activity of new 2-5A analogs

AUTHOR(S): Pauwels, R.; De Clercq, E.; Balzarini, J.; Sawai, H.; Imbach, J. L.; Gosselin, G.; Huss, S.; Reese, C. B.; Serafinowska, H.; et al.

CORPORATE SOURCE: Rega Inst. Med. Res., Univ. Leuven, Louvain, B-3000, Belg.

SOURCE: Chemica Scripta (1986), 26(1), 141-5

CODEN: CSRPB9; ISSN: 0004-2056

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Of a series of newly synthesized 2'-5' oligoadenylate (2-5A) analogs (with modifications in the ribose-phosphate backbone), several compds. proved effective as antimitogenic and antiproliferative agents. The antimitogenic activity was based upon the inhibition of DNA and protein synthesis in synchronized (serum-starved) Balb/c 3T3 cells, whereas the antiproliferative activity was detd. by monitoring the inhibition of murine leukemia L1210 cell growth. The antiproliferative effects of 2-5 A analogs correlated closely with their inhibitory effects on DNA and protein synthesis. When considered on a monomer equiv. basis, the mixed adenosine-cordycepin (1:2) cotrimer was more active than the cordycepin monomer, the phosphoramidate-linked adenosine trimer was less active than the aminoadenosine monomer, whereas the aristeromycin trimer, the xyloadenosine tri- and tetramers and the mixed adenosine-xyloadenosine (1:2, 2:1, 2:2, 1:3) tri- or tetramers were about equally active as either

the aristeromycin or xyloadenosine monomer. It is likely that the latter 2-5A analogs owe their biol. activity to degradn. to their monomer units.

IT 85818-47-9 103998-32-9

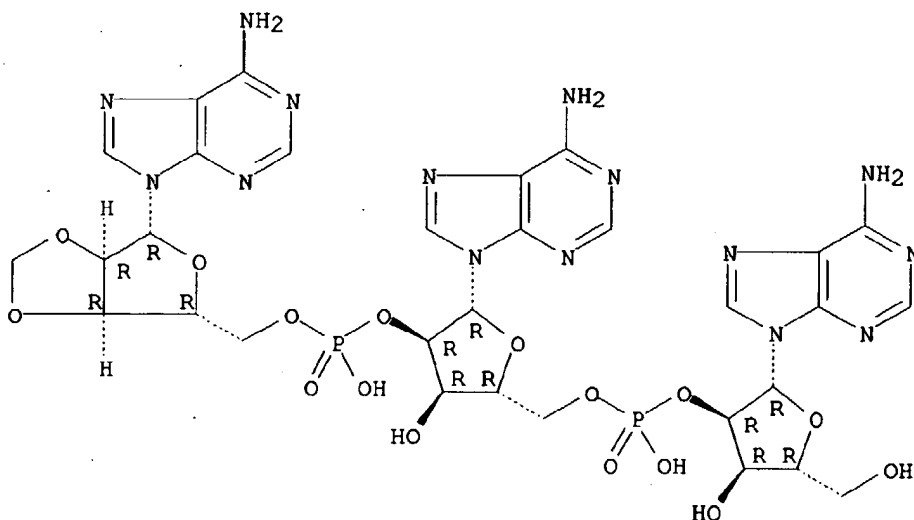
RL: BIOL (Biological study)

(DNA and protein synthesis response to)

RN 85818-47-9 HCAPLUS

CN Adenosine, adenylyl-(2'.fwdarw.5')-adenylyl-(2'.fwdarw.5')-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

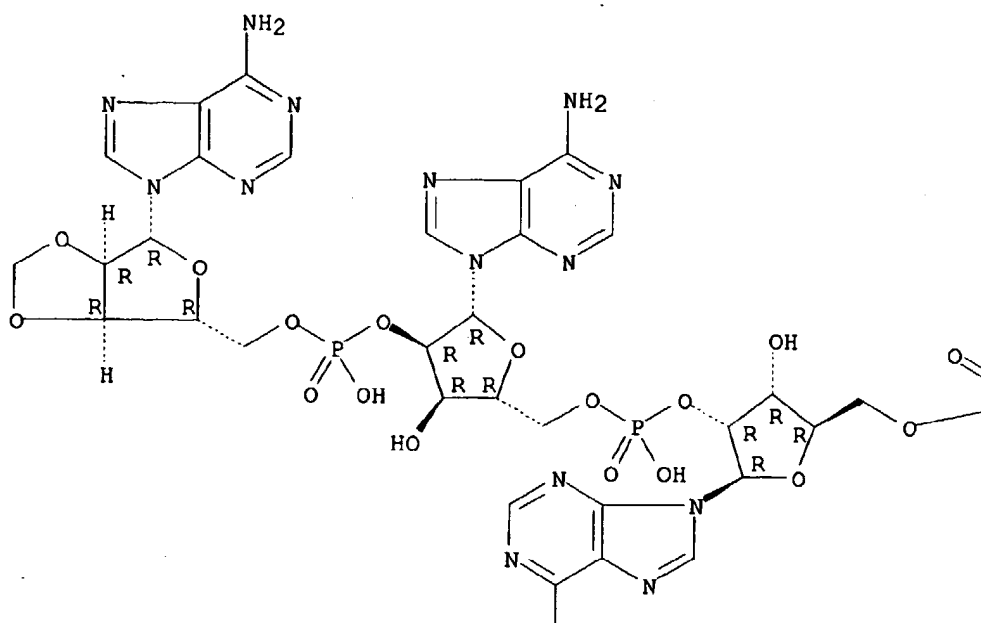


RN 103998-32-9 HCAPLUS

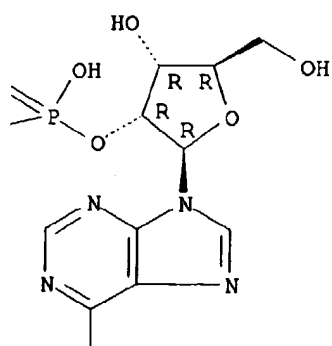
CN Adenosine, adenylyl-(2'.fwdarw.5')-adenylyl-(2'.fwdarw.5')-adenylyl-(2'.fwdarw.5')-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



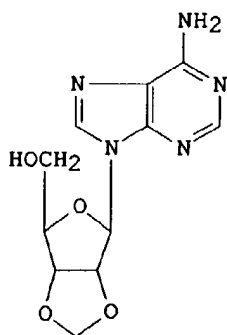
PAGE 2-A

|
NH₂

PAGE 2-B

|
NH₂

L30 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:130202 HCAPLUS
DOCUMENT NUMBER: 104:130202
TITLE: 2',3'-O-Methylene derivatives of ribonucleosides
AUTHOR(S): Norman, David G.; Reese, Colin B.; Serafinowska, Halina T.
CORPORATE SOURCE: Dep. Chem., King's Coll., Strand/London, WC2R 2LS, UK
SOURCE: Synthesis (1985), (8), 751-4
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:130202
GI



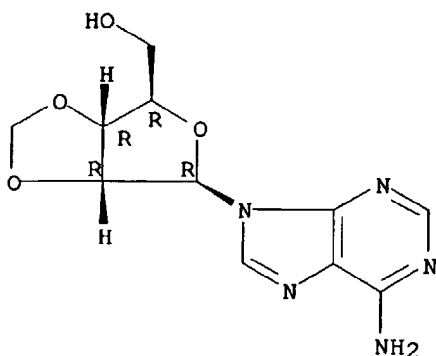
II

- AB 5'-O,N6-Ditrityladenosine (I), prepd. from adenosine, was refluxed with CH₂Br₂, NaOH, CH₂Cl₂, H₂O, and cetyltrimethylammonium bromide and the product was detritylated with AcOH-H₂O at reflux to give methyleneadenosine II (yield 50% based on I). Analogous methylenation of 5'-O-trityluridine gave 2',3'-O-methylene-5'-O-trityluridine (III) which was detritylated to give 2',3'-O-methyleneuridine. Also prepd. was N4-benzoyl-2',3'-O-methylenecytidine from III.
- IT 4137-31-9P 101072-38-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and tritylation of)

RN 4137-31-9 HCAPLUS

CN Adenosine, 2',3'-O-methylene- (7CI, 8CI, 9CI) (CA INDEX NAME)

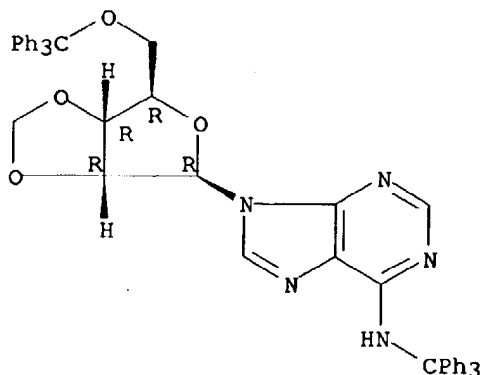
Absolute stereochemistry.



RN 101072-38-2 HCAPLUS

CN Adenosine, 2',3'-O-methylene-N-(triphenylmethyl)-5'-O-(triphenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L30 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1983:213907 HCAPLUS

DOCUMENT NUMBER: 98:213907

TITLE: Analogs and analog inhibitors of ppp(A2'p)nA. Their stability and biological activity

AUTHOR(S): Haugh, Margaret C.; Cayley, P. Jane; Serafinowska, Halina T.; Norman, David G.; Reese, Colin B.; Kerr, Ian M.

CORPORATE SOURCE: Imp. Cancer Res. Fund Lab., London, UK

SOURCE: European Journal of Biochemistry (1983), 132(1), 77-84
CODEN: EJBICAI; ISSN: 0014-2956

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Higher oligomers of ppp(A2'p)nA (n = 2-6) together with (A2'p)nA,

(A2'p)2A3'OCH₃, (A2'p)2A2',3'CH₂, (A2'p)2dA, dA2'p)2dA, their 5'-monophosphates and diphosphates and 5'-S-methylphosphorothioates have been investigated for relative stability and biol. activity in mouse and human cells and mouse, human, and rabbit cell-free systems. The oligomers from trimer to heptamer inhibited protein and DNA synthesis when introduced into intact mouse cells and activated the ppp(A2'p)nA-dependent RNase at below nanomolar concns. in mouse cell exts. The 5'-diphosphates pp(A2'p)2A and corresponding analogs were active both in cell-free systems and on introduction into intact cells. The exception to this was the all 3'-deoxyadenosine analog pp(dA2'p)2dA which failed to activate the ppp(A2'p)nA-dependent nuclease in the mouse L and human (Daudi and HeLa) cell exts. tested. Of the active analogs the 3'-OCH₃ appeared to be the most stable in the cells and systems employed. On the other hand the non-phosphorylated 'core' (A2'p)2A and its 3'-substituted analogs were inactive in mouse L and Ehrlich ascites tumor cell-free systems and had no effect on intact (nonpermeabilized) 3T3 cells. In intact mouse L cells or exts. from interferon-treated human (Daudi) cells, the 5'-monophosphate, p(A2'p)2A mimicked the action of ppp(A2'p)2A, possibly through conversion to the 5'-diphosphate or 5'-triphosphate. The 5'-S-methylphosphorothioate derivs. of the 3'-substituted analogs are both more stable to exonucleolytic cleavage and unlikely to be converted to the 5'-diphosphates or 5'-triphosphates. They are analog inhibitors of ppp(A2'p)nA in mouse L cell exts. How widely they will be effective in a variety of cell-free systems and intact cells remains to be established. The 5'-diphosphate pp(A2'p)2A and corresponding analogs were not equally active, nor was the 5'-S-methylphosphorothioate [CH₃Sp(A2'p)2A2',3'CH₂] equally effective as an analog inhibitor, in different cell-free systems. This emphasizes the apparent differences in the properties of the ppp(A2'p)nA-dependent RNases from different sources. Accordingly, in looking for a generally effective analog inhibitor of ppp(A2'p)2A its activity in a variety of exts. should be tested, and in any search for further analogs for potential clin. use, human cells and exts. should be employed.

IT 85818-42-4 85818-43-5 85818-47-9
85856-74-2

RL: BIOL (Biological study)

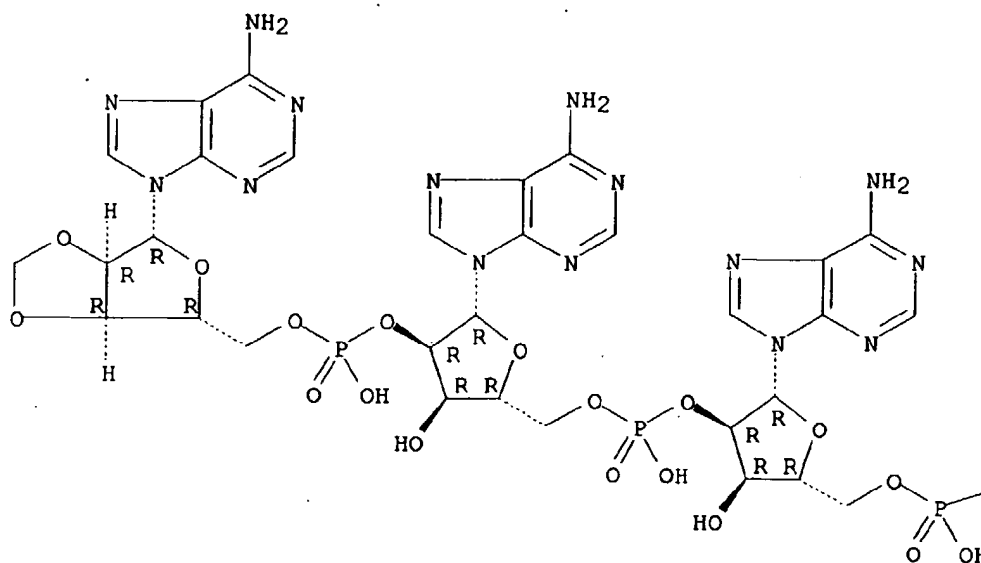
(stability and biol. activity of, RNase activation in relation to, in human and lab. animal system)

RN 85818-42-4 HCAPLUS

CN Adenosine, 5'-O-[hydroxy(phosphonooxy)phosphinyl]adenylyl-(2'.fwdarw.5')-adenylyl-(2'.fwdarw.5')-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



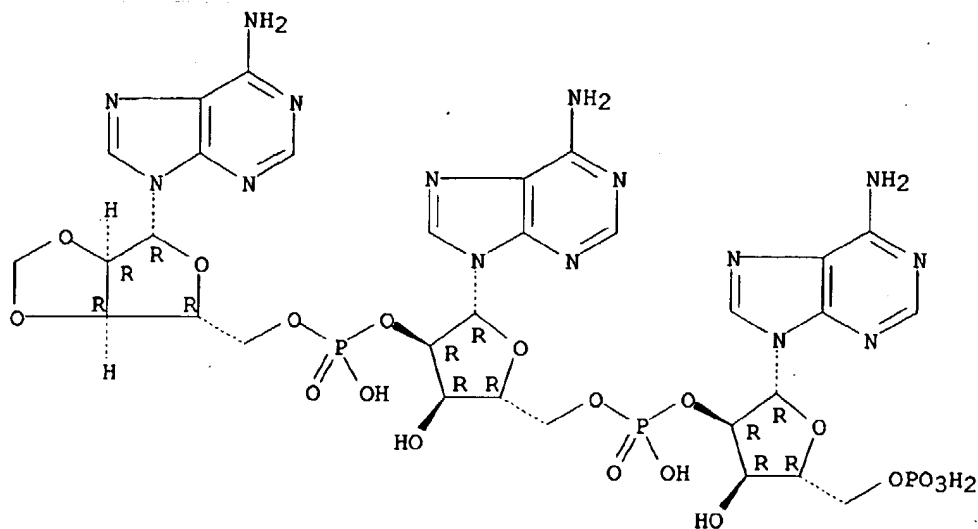
PAGE 1-B

—OPO₃H₂

RN 85818-43-5 HCAPLUS

CN Adenosine, 5'-O-phosphonoadenylyl-(2'.fwdarw.5')-adenylyl-(2'.fwdarw.5')-2',3'-O-methylene- (9CI) (CA INDEX NAME)

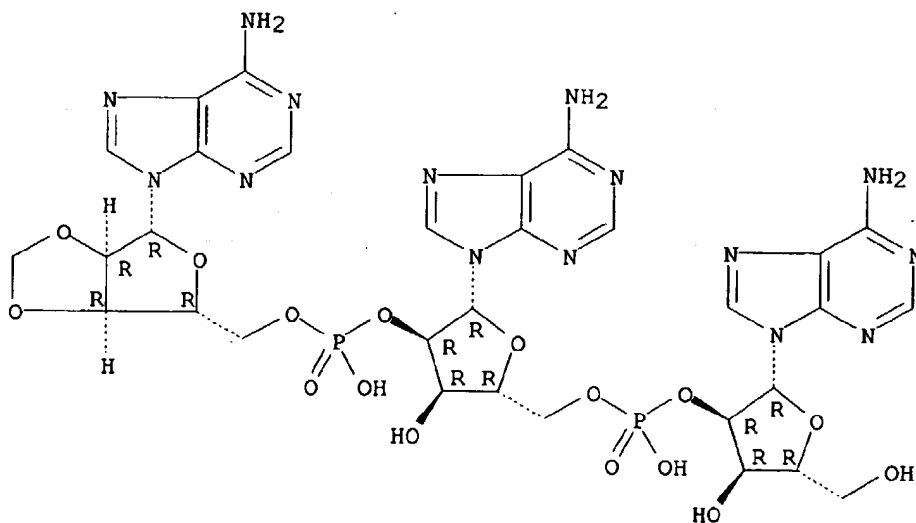
Absolute stereochemistry.



RN 85818-47-9 HCAPLUS

CN Adenosine, adenylyl-(2'.fwdarw.5')-adenylyl-(2'.fwdarw.5')-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

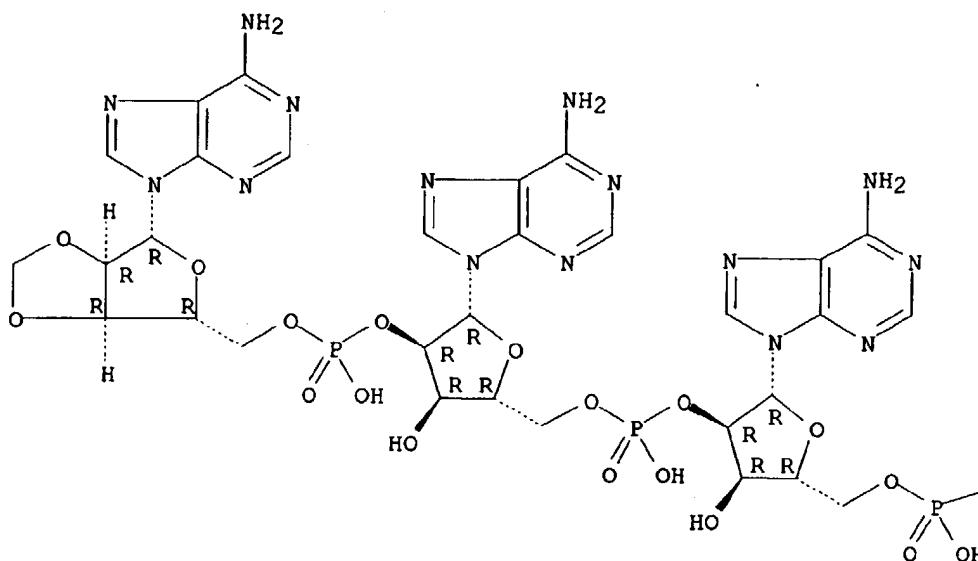


RN 85856-74-2 HCAPLUS

CN Adenosine, 5'-O-[hydroxy(methylthio)phosphinyl]adenylyl-(2'.fwdarw.5')-adenylyl-(2'.fwdarw.5')-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

—SMe

L30 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1979:168881 HCAPLUS
 DOCUMENT NUMBER: 90:168881
 TITLE: 4'-Substituted nucleosides. 5. Hydroxymethylation of
 nucleoside 5'-aldehydes
 AUTHOR(S): Jones, Gordon H.; Taniguchi, Masao; Tegg, Derek;
 Moffatt, John G.
 CORPORATE SOURCE: Inst. Mol. Biol., Syntex Res., Palo Alto, CA, USA
 SOURCE: Journal of Organic Chemistry (1979), 44(8), 1309-17

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Crossed aldol condensation between variously substituted nucleoside 5'-aldehydes and HCHO in the presence of aq. NaOH led, following rate-limiting Cannizzaro redn., to the corresponding 4'-hydroxymethylnucleoside derivs. The speed and overall efficiency of the above reactions were improved by incorporating a borohydride redn. of the initial aldol product rather than relying upon the normal Cannizzaro redn. Such reactions conducted with 2',3'-unsubstituted nucleoside 5'-aldehydes gave mixts. of 4'-hydroxymethylnucleosides epimeric at C-3', presumably via a reverse aldol cleavage followed by recyclization. Hence the use of base stable 2',3'-O-protecting groups is recommended for these reactions. In the case of 2',3'-O-isopropylidene derivs. of N6-benzoyladenine and N4-benzoylcytidine 5'-aldehydes, some exchange of the acetonide by a methylene group was obsd. and mechanism is proposed. For extension to the 2'-deoxynucleoside series, the corresponding hydroxymethylation of 3'-O-benzylthymidine 5'-aldehyde followed by catalytic hydrogenolysis led to 4'-hydroxymethylthymidine. Synthesis of a no. of new, variously protected nucleoside 5'-aldehydes are described.

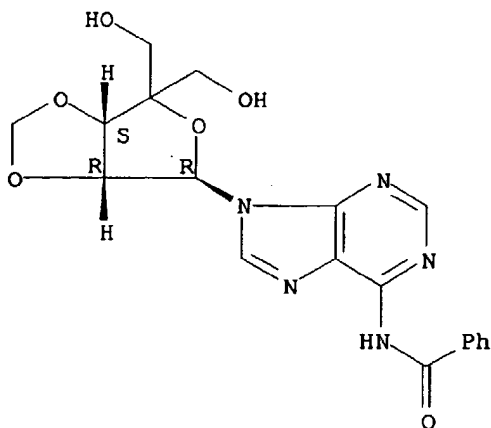
IT 63592-94-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 63592-94-9 HCAPLUS

CN Adenosine, N-benzoyl-4'-C-(hydroxymethyl)-2',3'-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L30 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1977:453510 HCAPLUS

DOCUMENT NUMBER: 87:53510

TITLE: Synthetic routes to 4'-hydroxymethylnucleosides

AUTHOR(S): Youssefhey, R.; Tegg, D.; Verheyden, J. P. H.; Jones, G. H.; Moffatt, J. G.

CORPORATE SOURCE: Inst. Mol. Biol., Syntex Res., Palo Alto, CA, USA

SOURCE: Tetrahedron Letters (1977), (5), 435-8

CODEN: TELEAY; ISSN: 0040-4039

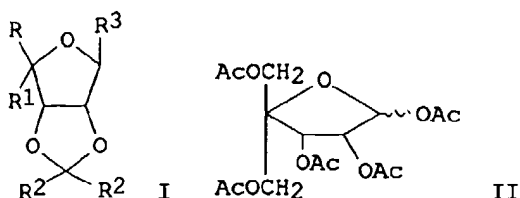
DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI



AB The aldehydes I ($R = \text{CHO}$, $R_1 = \text{H}$) [$R_2 = (\text{CH}_2)_5$, $R_3 = \text{uracil}$; $R_2 = \text{Me}$, $R_3 = \text{N}^6\text{-benzoyladenine}$] on treatment with HCHO and aq. NaOH at room temp. gave 38-9% I ($R = R_1 = \text{CH}_2\text{OH}$, R_2 , R_3 as before) which on hydrolysis with 9:1 $\text{CF}_3\text{CO}_2\text{H}-\text{H}_2\text{O}$ gave the unprotected 4'-hydroxymethyl nucleosides. The acetoxymethyl compd. II, prepd. from 3-O-benzyl-1,2-O-isopropylidene- α -D-allofuranose by sequential NaIO_4 oxidn., condensation with HCHO and aq. NaOH at 20.degree. for 4 days, hydrogenolysis, acetylation, and acetolysis, condensed with a variety of heterocyclic bases. E.g., II with chloropurine in MeCN at 55.degree. for 2 h in the presence of $\text{Hg}(\text{CN})_2$ and SnCl_4 gave 84% 9-(4-acetoxymethyl-2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-6-chloropurine which with $\text{NH}_3(1)$ gave 4'-hydroxymethyladenosine.

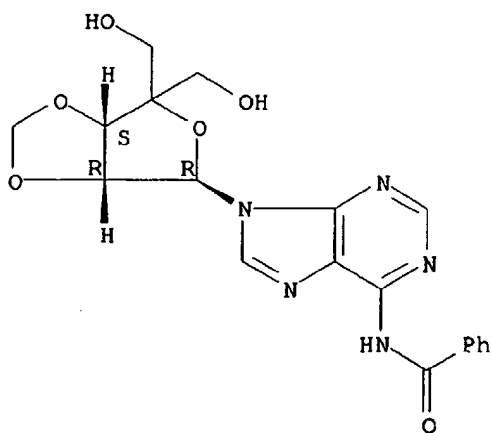
IT 63592-94-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 63592-94-9 HCAPLUS

CN Adenosine, N-benzoyl-4'-C-(hydroxymethyl)-2',3'-O-methylene- (9CI) (CA
INDEX NAME)

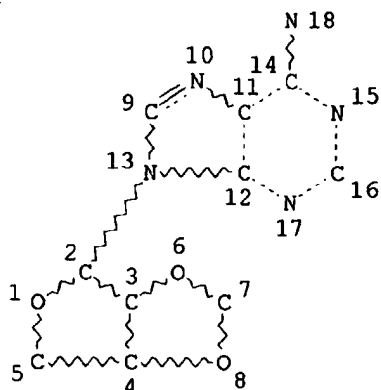
Absolute stereochemistry.



=> d que

L1

STR



NODE ATTRIBUTES:

NSPEC IS RC AT 18
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

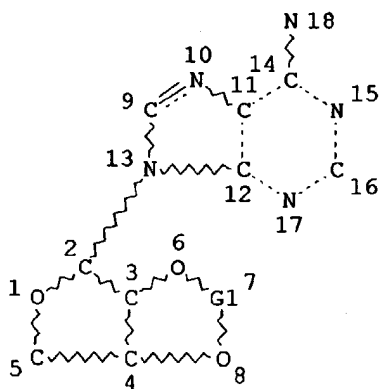
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L2 3214 SEA FILE=REGISTRY SSS FUL L1

L5 STR



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 19 @20 21

Ak~C~Cb
 22 @23 24

Cb~C~Cb
 25 @26 27

VAR G1=20/23/26

NODE ATTRIBUTES:

NSPEC IS RC AT 18
 CONNECT IS E1 RC AT 19
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L6 2399 SEA FILE=REGISTRY SUB=L2 SSS FUL L5
L31 1068 SEA FILE=HCAPLUS ABB=ON PLU=ON L6

=> d-ibib abs hitstr-1-3-500-502-1066-1068

L31 ANSWER 1 OF 1068 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:831353 HCAPLUS
DOCUMENT NUMBER: 138:73419
TITLE: Gel formation properties of a uracil-appended
cholesterol gelator and cooperative effects of the
complementary nucleobases
AUTHOR(S): Snip, Erwin; Koumoto, Kazuya; Shinkai, Seiji
CORPORATE SOURCE: Chemotransfiguration Project, Japan Science and
Technology Corporation (JST), Kurume, Fukuoka,
839-0861, Japan
SOURCE: Tetrahedron (2002), 58(43), 8863-8873
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

*Large # of hits
only a few printed*

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The authors designed and synthesized a uracil-appended cholesterol gelator I in order to control the gel stability and the gel morphol. by addn. of the complementary and non-complementary nucleobase derivs. Compd. I forms columnar stacks in cyclohexane due to the van der Waals interaction (cholesterol-cholesterol interaction) and the intergelator hydrogen bonding between uracil moieties. Addn. of a 'monomeric' adenosine, II, into the gel only decreases the stability with increasing the concn. The destabilization is ascribed to a lack of intergelator hydrogen bonding accompanied with forming the complementary base pairs between I and II. In contrast, addn. of an adenine-appended cholesterol induces a different behavior; with increasing concn. the mixed gel is initially stabilized and then destabilized, giving rise to a max. at the ratio of I/adenine-appended cholesterol = 1:1 for the Tgel plot. One may consider, therefore, that when the additive has a common, column-forming cholesterol

moiety, the cholesterol-cholesterol interaction can operate cooperatively with the complementary base pairing. In addn., the gel fiber structure is clearly changed by the addn. of the adenine-appended cholesterol. Taking the fact that there is no report for such an additive effect inducing a structural change with maintaining the gel stability into consideration, the authors' attempt at combining cholesterol columnar stacks with the nucleobase additives provides a new methodol. to control the stability and the morphol. of organogels.

IT 213552-31-9P

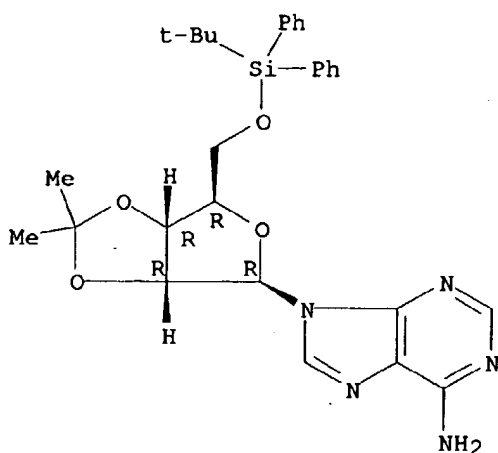
RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of uracil-appended cholesterol gelator and effects on gel stability and morphol. using complementary and non-complementary nucleobases)

RN 213552-31-9 HCAPLUS

CN Adenosine, 5'-O-[(1,1-dimethylethyl)diphenylsilyl]-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 362-75-4, 2',3'-O-Isopropylidene adenosine

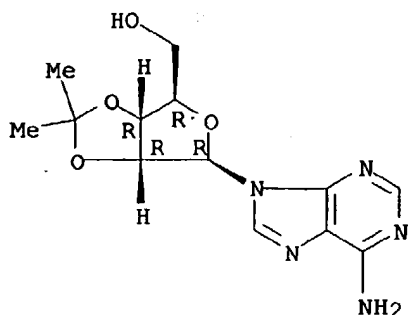
RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of uracil-appended cholesterol gelator and effects on gel stability and morphol. using complementary and non-complementary nucleobases)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 2 OF 1068 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 2002:816750 HCAPLUS
 DOCUMENT NUMBER: 138:39493
 TITLE: Adenosine 5'-O-(1-Boranotriphosphate) Derivatives as Novel P2Y1 Receptor Agonists
 AUTHOR(S): Nahum, Victoria; Zuendorf, Gregor; Levesque, Sebastien A.; Beaudoin, Adrien R.; Reiser, Georg; Fischer, Bilha
 CORPORATE SOURCE: Department of Chemistry Gonda-Goldschmied Medical Research Center, Bar-Ilan University, Ramat-Gan, 52900, Israel
 SOURCE: Journal of Medicinal Chemistry (2002), 45(24), 5384-5396
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:39493

AB P2-receptors (P2-Rs) represent important targets for novel drug development. Most ATP analogs proposed as potential drug candidates have short-comings such as limited receptor-selectivity and limited stability that justify the search for new P2-R agonists. Therefore, a novel series of nucleotides based on the adenosine 5'-O-(1-boranotriphosphate) (ATP-.alpha.-B) scaffold was developed and tested as P2Y1-R agonists. An efficient four-step one-pot synthesis of several ATP-.alpha.-B analogs from the corresponding nucleosides was developed, as well as a facile method for the sepn. of the diastereoisomers (A and B isomers) of the chiral products. The potency of the new analogs as P2Y1-R agonists was evaluated by the agonist-induced Ca²⁺ release of HEK 293 cells stably transfected with rat-brain P2Y1-R. ATP-.alpha.-B A isomer was equipotent with ATP (EC₅₀ = 2 .times. 10⁻⁷ M). However, 2-MeS- and 2-Cl- substitutions on ATP-.alpha.-B (A isomer) increased the potency of the agonist up to 100-fold, with EC₅₀ values of 4.5 .times. 10⁻⁹ and 3.6 .times. 10⁻⁹ M, compared to that of the ATP-.alpha.-B (A isomer). Diastereoisomers A of all ATP-.alpha.-B analogs were more potent in inducing Ca²⁺ release than the corresponding B counterparts, with a 20-fold difference for 2-MeS-ATP-.alpha.-B analogs. The chem. stability of the new P2Y1-R agonists was evaluated by 31P NMR under physiol. and gastric-juice pH values at 37 .degree.C, with rates of hydrolysis of 2-MeS-ATP-.alpha.-B of 1.38 .times. 10⁻⁷ s⁻¹ (t_{1/2} of 1395 h) and 3.24 .times. 10⁻⁵ s⁻¹ (t_{1/2} = 5.9 h), resp. The enzymic stability of the new analogs toward spleen NTPDase was evaluated. Most of the new analogs were

poor substrates for the NTPDase, with ATP-.alpha.-B (A isomer) hydrolysis being 5% of the hydrolysis rate of ATP. Diastereoisomers A and B exhibited different stability, with A isomers being significantly more stable, up to 9-fold. Furthermore, A isomers that are potent P2Y1-R agonists barely interact with NTPDase, thus exhibiting protein selectivity. Therefore, on the basis of our findings, the new, highly water-sol., P2Y1-R agonists may be considered as potentially promising drug candidates.

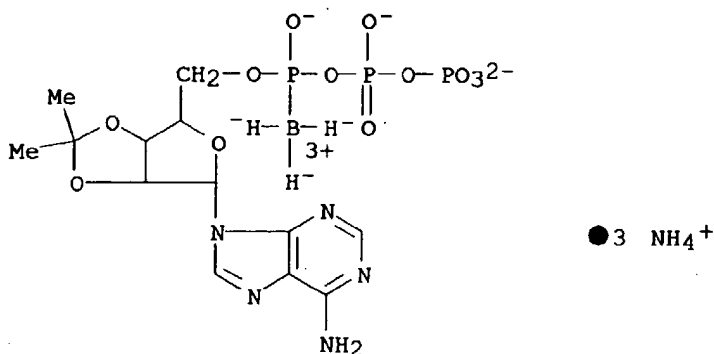
IT 478867-98-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of adenosine boranotriphosphate derivs. as novel P2Y1 receptor agonists)

RN 478867-98-0 HCAPLUS

CN Borate(4-), trihydro[2',3'-O-(1-methylethylidene)adenosine 5'.fwdarw.P-[triphosphato(III,V,V)-.kappa.P](4-)]-, triammonium hydrogen, (T-4)- (9CI) (CA INDEX NAME)



● H⁺

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 3 OF 1068 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:789678 HCAPLUS

DOCUMENT NUMBER: 138:24909

TITLE: Synthesis and Evaluation of Analogs of 5'-([(Z)-4-Amino-2-butenyl]methylamino)-5'-deoxyadenosine as Inhibitors of Tumor Cell Growth, Trypanosomal Growth, and HIV-1 Infectivity

AUTHOR(S): Marasco, Canio J., Jr.; Kramer, Debora L.; Miller, John; Porter, Carl W.; Bacchi, Cyrus J.; Rattendi, Donna; Kucera, Louis; Iyer, Nathan; Bernacki, Ralph; Pera, Paula; Sufrin, Janice R.

CORPORATE SOURCE: Grace Cancer Drug Center, Department of Pharmacology and Therapeutics, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(23), 5112-5122

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:24909

AB A well-defined series of 5'-([2]-4-amino-2-butenyl)methylamino)-5'-deoxyadenosine analogs was designed and synthesized in order to further ascertain the optimal structural requirements for S-adenosylmethionine decarboxylase inhibition and potentially to augment and perhaps sep. their antiproliferative and antitrypanosomal activities. Most structural modifications had a deleterious affect on both the antitrypanosomal and antineoplastic activity of 5'-([2]-4-amino-2-butenyl)methylamino)-5'-deoxyadenosine. However, di-O-acetylation of the parent compd. produced a potential prodrug that caused markedly pronounced inhibition of trypanosomal and neoplastic cell growth and viability. Moreover, the acetylated deriv. of 5'-([2]-4-amino-2-butenyl)methylamino)-5'-deoxyadenosine did inhibit HIV-1 growth and infectivity, whereas the parent compd. did not.

IT 478161-16-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

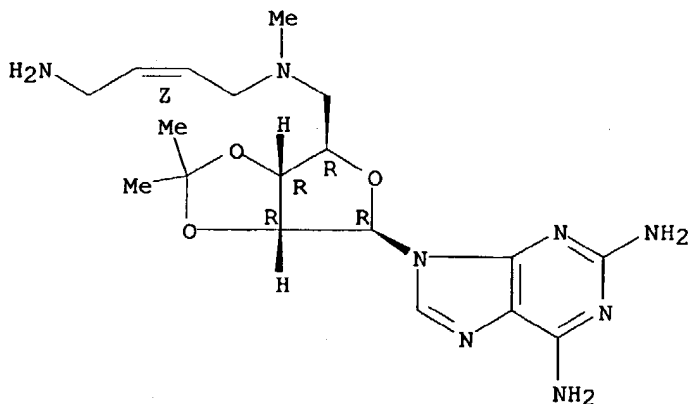
(synthesis and evaluation of analogs of aminobutenylmethylaminodeoxyadenosine as inhibitors of tumor cell growth trypanosomal growth and HIV infectivity)

RN 478161-16-9 HCAPLUS

CN Adenosine, 2-amino-5'-[[(2Z)-4-amino-2-butenyl)methylamino]-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 362-75-4 24514-56-5

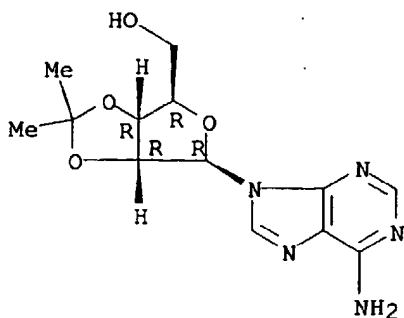
RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and evaluation of analogs of aminobutenylmethylaminodeoxyadenosine as inhibitors of tumor cell growth trypanosomal growth and HIV infectivity)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

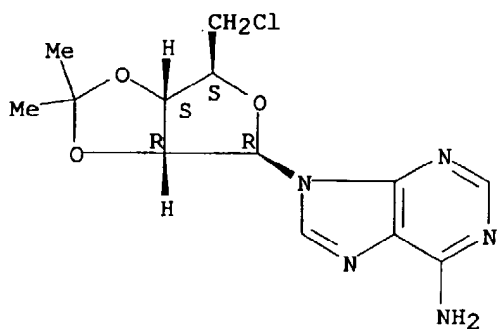
Absolute stereochemistry.



RN 24514-56-5 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 30685-38-2P 34245-49-3P 478161-08-9P

478161-09-0P 478161-10-3P 478161-11-4P

478161-13-6P 478161-14-7P 478161-15-8P

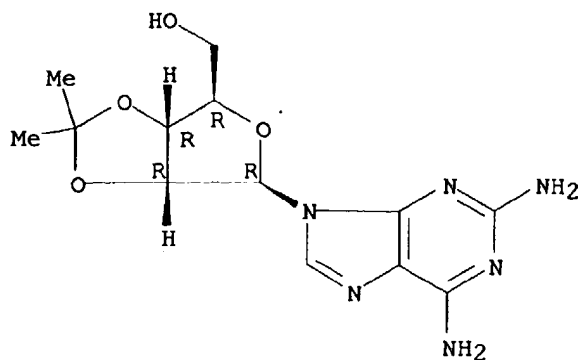
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and evaluation of analogs of aminobutenylmethylaminodeoxyadenosine as inhibitors of tumor cell growth trypanosomal growth and HIV infectivity)

RN 30685-38-2 HCAPLUS

CN Adenosine, 2-amino-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

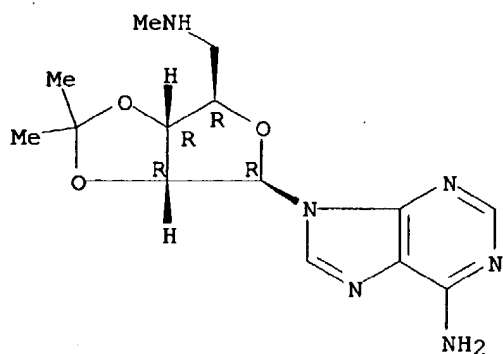
Absolute stereochemistry.



RN 34245-49-3 HCAPLUS

CN Adenosine, 5'-deoxy-5'-(methylamino)-2',3'-O-(1-methylethylidene)- (9CI)
(CA INDEX NAME)

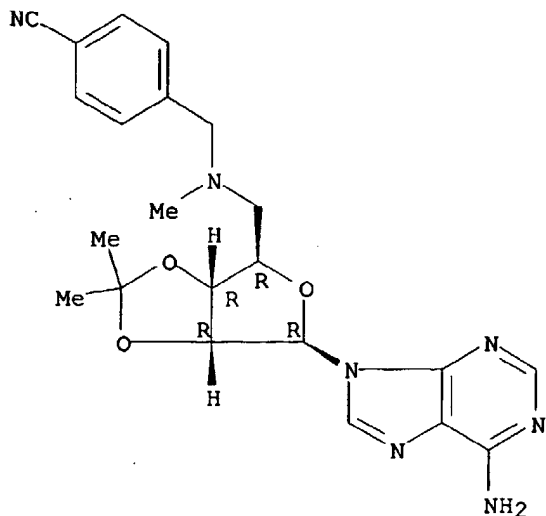
Absolute stereochemistry.



RN 478161-08-9 HCAPLUS

CN Adenosine, 5'-[[[4-cyanophenyl)methyl]methylamino]-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

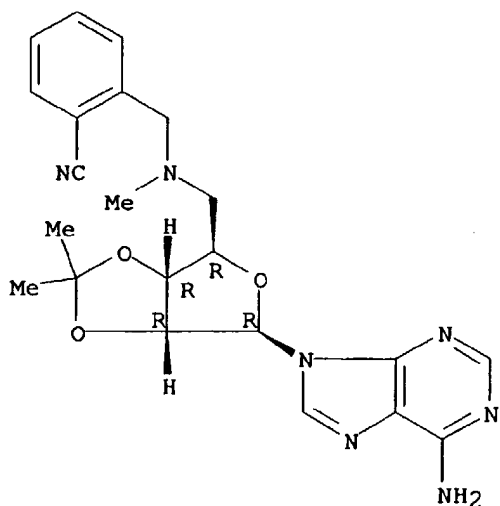
Absolute stereochemistry.



RN 478161-09-0 HCAPLUS

CN Adenosine, 5'-[[[(2-cyanophenyl)methyl]methylamino]-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

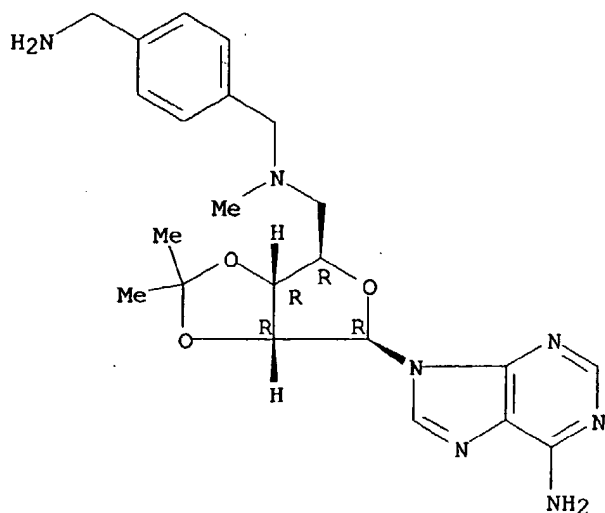
Absolute stereochemistry.



RN 478161-10-3 HCAPLUS

CN Adenosine, 5'-[[[4-(aminomethyl)phenyl]methyl]methylamino]-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

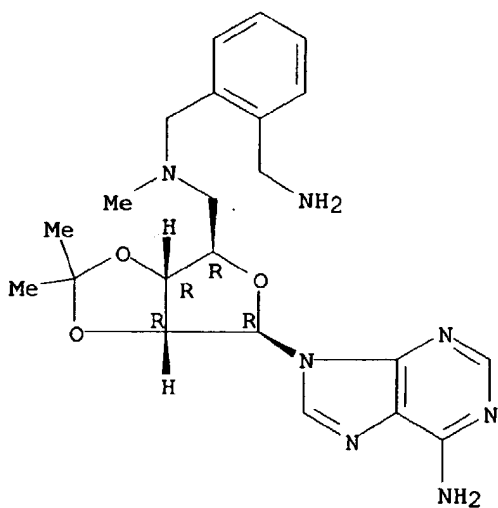
Absolute stereochemistry.



RN 478161-11-4 HCAPLUS

CN Adenosine, 5'-[[[2-(aminomethyl)phenyl]methyl]methylamino]-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

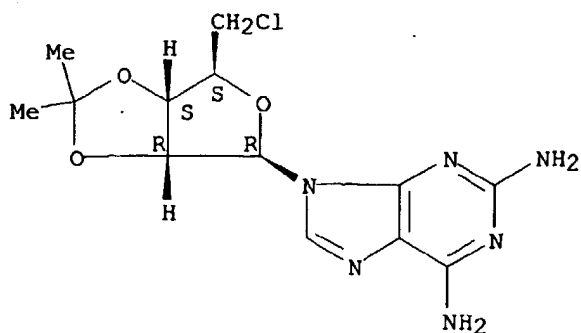
Absolute stereochemistry.



RN 478161-13-6 HCAPLUS

CN Adenosine, 2-amino-5'-chloro-5'-deoxy-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

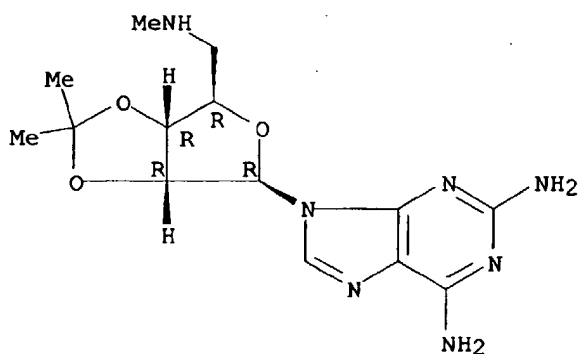
Absolute stereochemistry.



RN 478161-14-7 HCAPLUS

CN Adenosine, 2-amino-5'-deoxy-5'-(methylamino)-2',3'-O-(1-methylethylidene)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

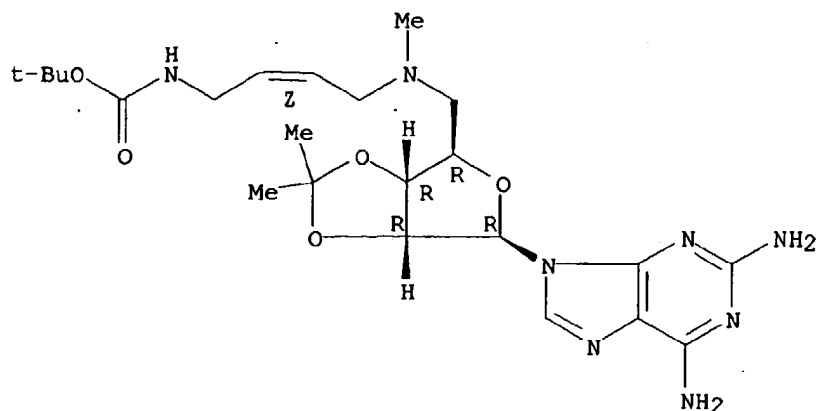


RN 478161-15-8 HCAPLUS

CN Adenosine, 2-amino-5'-deoxy-5'-[[(2Z)-4-[[(1,1-dimethylethoxy) carbonyl] amino]-2-butenyl]methylamino]-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

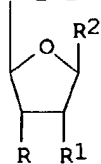
Double bond geometry as shown.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

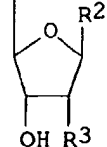
L31 ANSWER 500 OF 1068 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1986:497864 HCAPLUS
 DOCUMENT NUMBER: 105:97864
 TITLE: Synthesis and antiviral activity of certain nucleoside 5'-phosphonoformate derivatives
 AUTHOR(S): Vaghefi, Morteza M.; McKernan, Patricia A.; Robins, Roland K.
 CORPORATE SOURCE: Cancer Res. Cent., Brigham Young Univ., Provo, UT, 84602, USA
 SOURCE: Journal of Medicinal Chemistry (1986), 29(8), 1389-93
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:97864
 GI

CH₂O₂P(Cl)CO₂Et



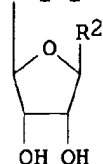
I

CH₂O₂P(OH)CO₂H



II

CH₂O₂P(OH)CONH₂



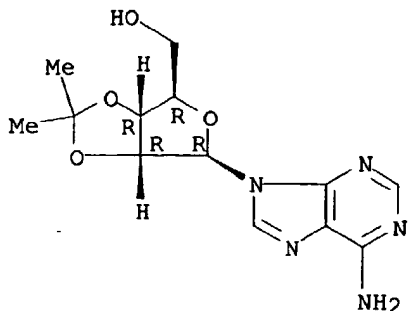
III

AB EtO₂CP(O)Cl₂ was prepd. and condensed with adenosine, guanosine, 2'-deoxyadenosine, and 2'-deoxyguanosine to yield nucleotides I (R,R₁ = OH; RR₁ = OMe₂O; R = OAc, R₁ = H; R₂ = adenine, guanine). Alk. treatment of I gave phosphonates II (R₃ = H, OH). Treatment of I (R,R₁ = OH) with NH₃-MeOH gave (aminocarbonyl)phosphonate III. II (R₃ = H, R₂ = adenine) exhibited the most potent antiviral activity of the group of nucleotides tested in vitro and was most active against herpes viruses, esp. HSV-2 (ED₅₀ = 40.μM). All of the compds. tested were nontoxic to confluent Vero cells at 10⁶ times 10³ μM.

IT 362-75-4

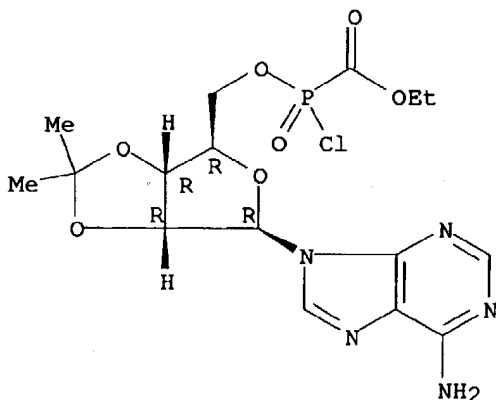
RL: RCT (Reactant); RACT (Reactant or reagent)
 (phosphorylation of)
 RN 362-75-4 HCAPLUS
 CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 102831-57-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and deisopropylidene of)
 RN 102831-57-2 HCAPLUS
 CN Adenosine, 2',3'-O-(1-methylethylidene)-, 5'-[(ethoxycarbonyl)phosphonochloridate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L31 ANSWER 501 OF 1068 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1986:479310 HCAPLUS
 DOCUMENT NUMBER: 105:79310
 TITLE: N6-Substituted deoxyribose analogs of adenosines
 INVENTOR(S): Hamilton, Harriet W.; Bristol, James A.; Moos, Walter;
 Trivedi, Bharat K.; Taylor, Michael; Patt, William C.
 PATENT ASSIGNEE(S): Warner-Lambert Co., USA
 SOURCE: Eur. Pat. Appl., 69 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent

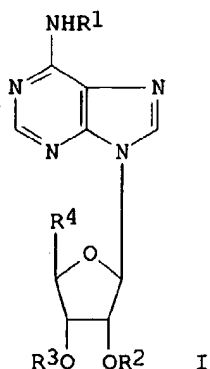
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 181129	A2	19860514	EP 1985-307717	19851025
EP 181129	A3	19870513		
EP 181129	B1	19890308		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AU 8548888	A1	19860508	AU 1985-48888	19851021
AU 575438	B2	19880728		
FI 8504153	A	19860427	FI 1985-4153	19851023
FI 81587	B	19900731		
FI 81587	C	19901112		
ZA 8508154	A	19860625	ZA 1985-8154	19851023
DK 8504884	A	19860427	DK 1985-4884	19851024
NO 8504278	A	19860428	NO 1985-4278	19851025
NO 165495	B	19901112		
NO 165495	C	19910220		
JP 61148194	A2	19860705	JP 1985-237759	19851025
ES 548238	A1	19861201	ES 1985-548238	19851025
AT 41158	E	19890315	AT 1985-307717	19851025
CA 1260931	A1	19890926	CA 1985-493849	19851025
CN 85108658	A	19860716	CN 1985-108658	19851026
CN 1013448	B	19910807		
ES 555142	A1	19871101	ES 1986-555142	19860520
PRIORITY APPLN. INFO.:			US 1984-665217	19841026
			US 1984-665232	19841026
			US 1984-665233	19841026
			US 1985-772315	19850906
			EP 1985-307717	19851025

GI



AB 5'-Deoxyadenosines I (R1 = cycloalkyl, CH₂CHPh₂, 1-indanyl, 1-tetralinyl, CHMeCH₂Ph, 1-naphthylmethyl; R2 and R3 are H, alkyl, alkanoyl, etc.; R4 = Me, halomethyl, CH₂SMe) were prepd., and they showed antipsychotic, antihypertensive, and analgesic activity. 6-(2,2-Diphenylethylamino)purine was treated with a 5-deoxyribose deriv. to give

I (R1 = CH₂CHPh₂, R2 = R3 = H, R4 = Me).

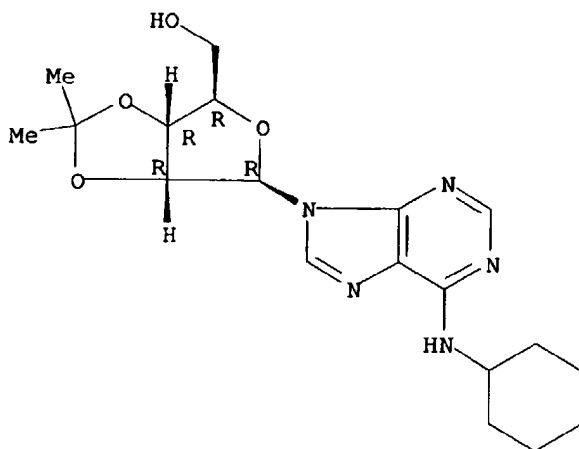
IT 3369-66-2P 103626-39-7P 103626-41-1P
 103626-42-2P 103626-44-4P 103626-45-5P
 103626-46-6P 103626-49-9P 103626-50-2P
 103626-51-3P 103626-53-5P 103626-58-0P
 103626-64-8P 103639-11-8P 103667-48-7P
 103729-37-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of)

RN 3369-66-2 HCAPLUS

CN Adenosine, N-cyclohexyl-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX
 NAME)

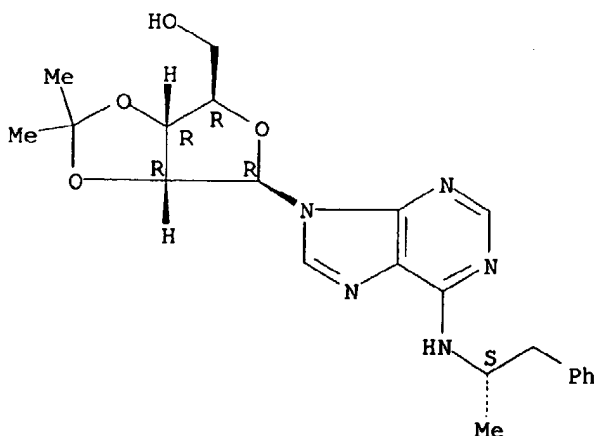
Absolute stereochemistry.



RN 103626-39-7 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)-N-(1-methyl-2-phenylethyl)-, (S)-
 (9CI) (CA INDEX NAME)

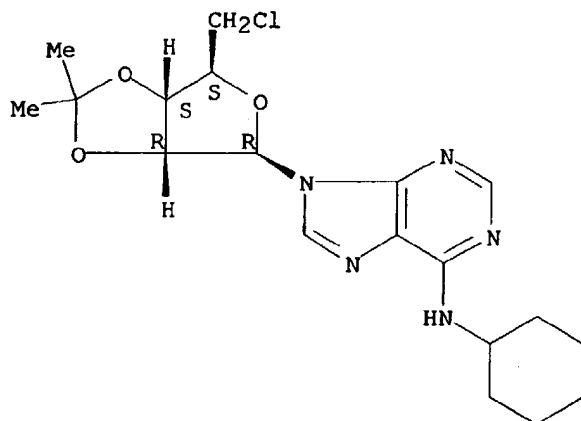
Absolute stereochemistry.



RN 103626-41-1 HCAPLUS

CN Adenosine, 5'-chloro-N-cyclohexyl-5'-deoxy-2',3'-O-(1-methylethylidene)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

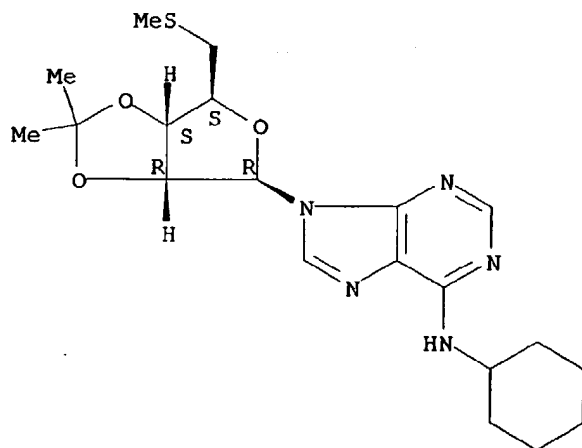


● HCl

RN 103626-42-2 HCAPLUS

CN Adenosine, N-cyclohexyl-5'-S-methyl-2',3'-O-(1-methylethylidene)-5'-thio- (9CI) (CA INDEX NAME)

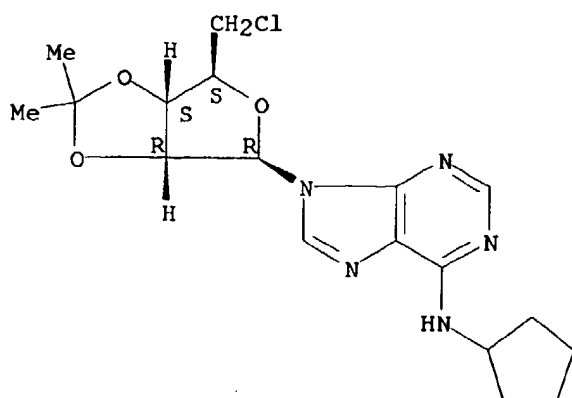
Absolute stereochemistry.



RN 103626-44-4 HCAPLUS

CN Adenosine, 5'-chloro-N-cyclopentyl-5'-deoxy-2',3'-O-(1-methylethylidene)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

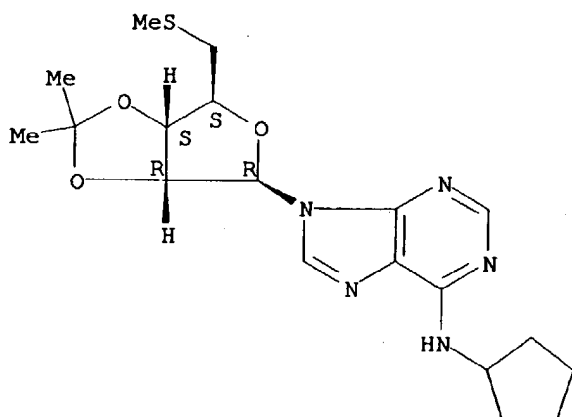


● HCl

RN 103626-45-5 HCAPLUS

CN Adenosine, N-cyclopentyl-5'-S-methyl-2',3'-O-(1-methylethylidene)-5'-thio-
(9CI) (CA INDEX NAME)

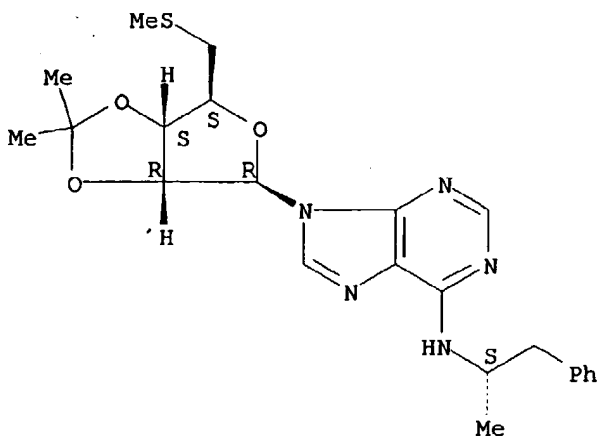
Absolute stereochemistry.



RN 103626-46-6 HCAPLUS

CN Adenosine, 5'-S-methyl-2',3'-O-(1-methylethylidene)-N-(1-methyl-2-
phenylethyl)-5'-thio-, (S)- (9CI) (CA INDEX NAME)

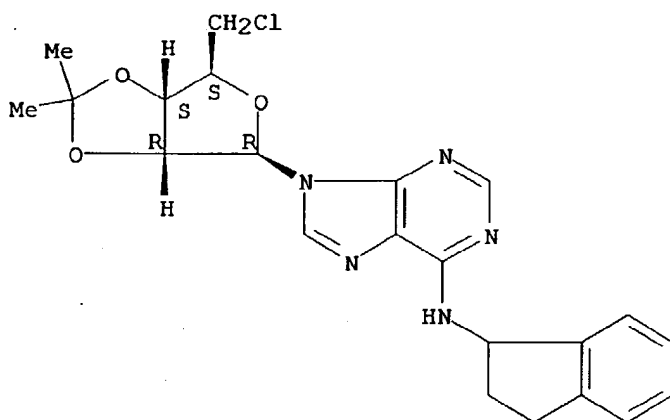
Absolute stereochemistry.



RN 103626-49-9 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-(2,3-dihydro-1H-inden-1-yl)-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

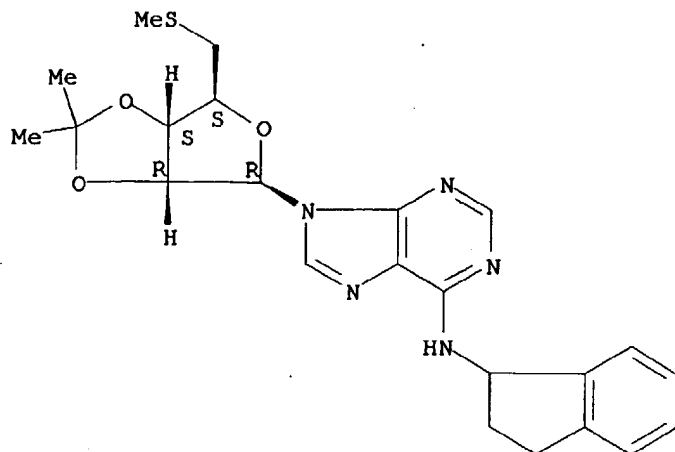
Absolute stereochemistry.



RN 103626-50-2 HCAPLUS

CN Adenosine, N-(2,3-dihydro-1H-inden-1-yl)-5'-S-methyl-2',3'-O-(1-methylethylidene)-5'-thio- (9CI) (CA INDEX NAME)

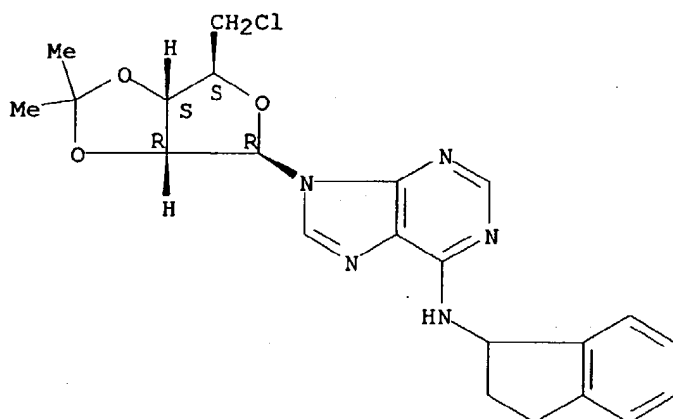
Absolute stereochemistry.



RN 103626-51-3 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-(2,3-dihydro-1H-inden-1-yl)-2',3'-O-(1-methylethylidene)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

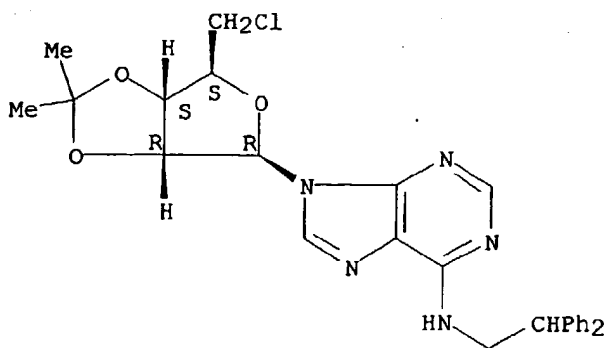


● HCl

RN 103626-53-5 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-(2,2-diphenylethyl)-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

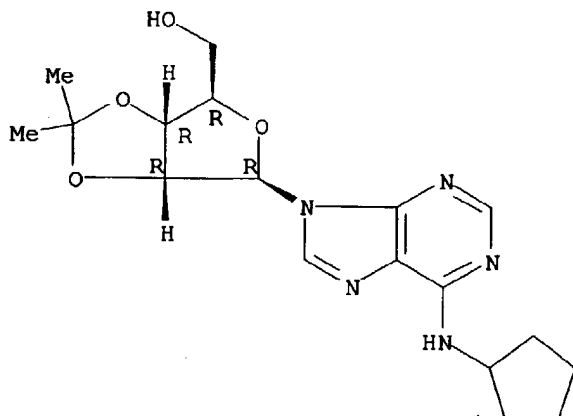
Absolute stereochemistry.



RN 103626-58-0 HCAPLUS

CN Adenosine, N-cyclopentyl-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

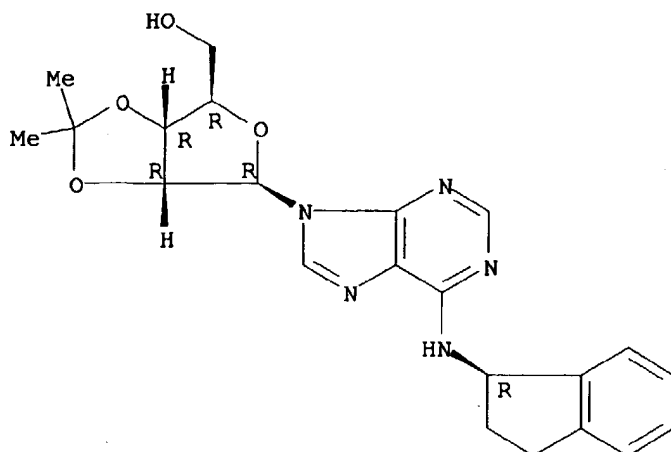
Absolute stereochemistry.



RN 103626-64-8 HCAPLUS

CN Adenosine, N-(2,3-dihydro-1H-inden-1-yl)-2',3'-O-(1-methylethylidene)-, (R)- (9CI) (CA INDEX NAME)

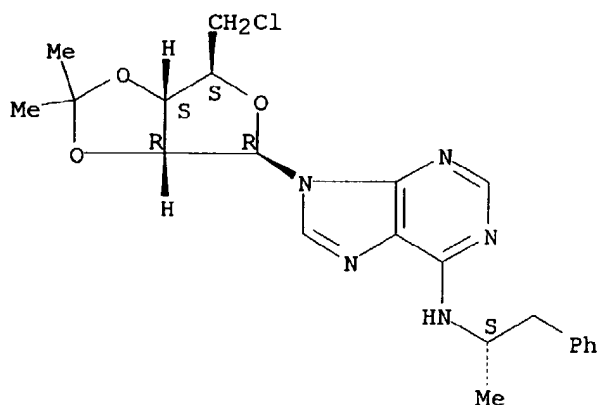
Absolute stereochemistry.



RN 103639-11-8 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-2',3'-O-(1-methylethylidene)-N-(1-methyl-2-phenylethyl)-, (S)- (9CI) (CA INDEX NAME)

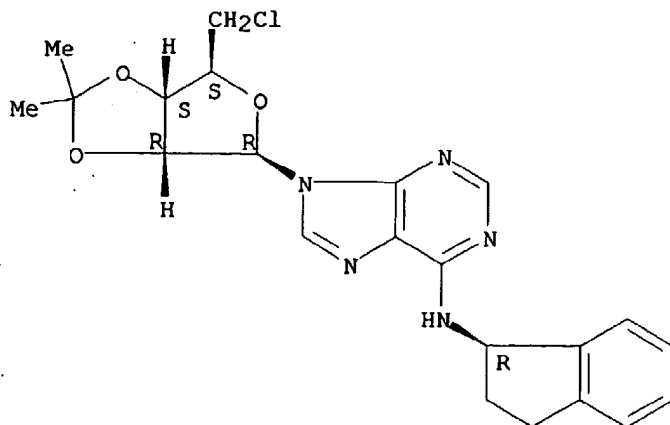
Absolute stereochemistry.



RN 103667-48-7 HCAPLUS

CN Adenosine, 5'-chloro-5'-deoxy-N-(2,3-dihydro-1H-inden-1-yl)-2',3'-O-(1-methylethylidene)-, (R)- (9CI) (CA INDEX NAME)

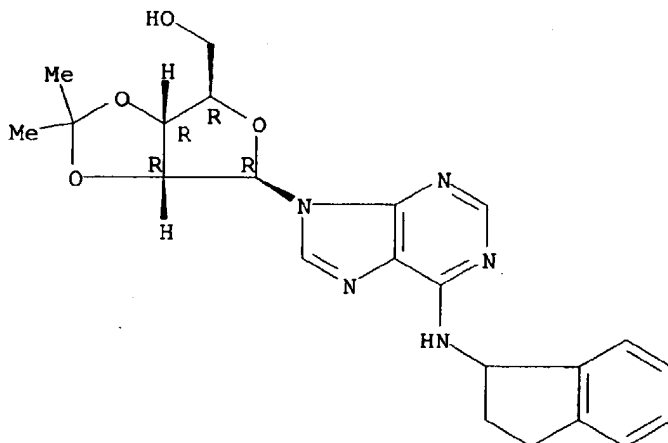
Absolute stereochemistry.



RN 103729-37-9 HCAPLUS

CN Adenosine, N-(2,3-dihydro-1H-inden-1-yl)-2',3'-O-(1-methylethylidene)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L31 ANSWER 502 OF 1068 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1986:474858 HCAPLUS

DOCUMENT NUMBER: 105:74858

TITLE: Mevalonate-5-diphosphate decarboxylase:
stereochemical course of ATP-dependent phosphorylation
of mevalonate 5-diphosphate

AUTHOR(S): Iyengar, Radha; Cardemil, Emilio; Frey, Perry A.

CORPORATE SOURCE: Dep. Quim., Univ. Santiago, Santiago, Chile

SOURCE: Biochemistry (1986), 25(16), 4693-8

CODEN: BICAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chicken liver mevalonate 5-diphosphate carboxylase catalyzes the reaction
of mevalonate 5-diphosphate (MVADP) with ATP to produce isopentenyl
diphosphate, ADP, CO₂, and inorg. phosphate. The overall reaction

involves an anti elimination of the tertiary hydroxyl and carboxyl groups. To investigate the mechanism for transfer of the terminal phosphoryl group of ATP to the C-3 O atom of MVADP, the reaction was carried out using stereospecifically labeled (SP)-adenosine 5'-O-(3-thio[3-1702,180]triphosphate) ([.gamma.-1702,180]ATP.gamma.S) in place of ATP. The configuration of the [170,180]thiophosphate produced was found to be RP, corresponding to overall inversion of configuration at the P atom in the thiophosphoryl group transfer step. This result was consistent with the direct transfer of the thiophosphoryl group from (SP)-[.gamma.-1702,180]ATP.gamma.S to MVADP at the active site. The result did not indicate the involvement of a covalent thiophosphoryl-enzyme on the reaction pathway.

IT 362-75-4

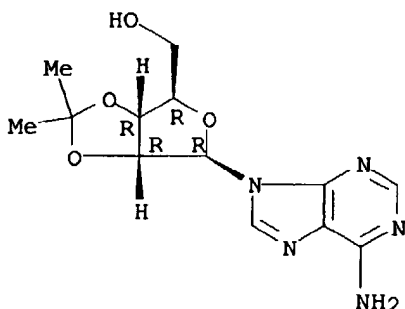
RL: PROC (Process).

(conversion of, to oxygen-18-labeled adenosine)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L31 ANSWER 1066 OF 1068 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1958:11156 HCAPLUS

DOCUMENT NUMBER: 52:11156

ORIGINAL REFERENCE NO.: 52:2027g-i,2028a-b

TITLE: Esters of adenosine with organic and inorganic acids

AUTHOR(S): Huber, Gerhard

CORPORATE SOURCE: Forschungslab. Zellstoff-Fabrik Waldhof, Mannheim-Waldhof, Germany

SOURCE: Chem. Ber. (Berlin) (1956), 89, 2853-62

DOCUMENT TYPE: Journal

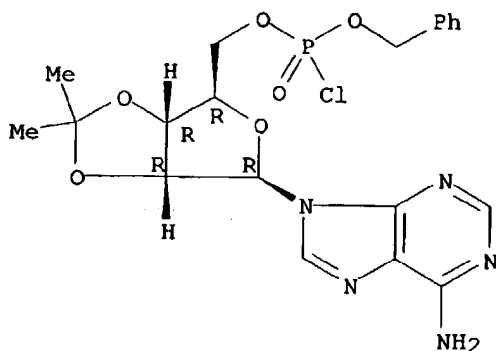
LANGUAGE: Unavailable

AB The m.p. and Rf value in H₂O-satd. BuOH were detd. for esters of adenosine (I). The 2',3'-isopropylidene deriv. of I (II) (Rf 0.60) (5 g.) and 30 ml. Ac₂O in 100 ml. C₅H₅N after 2 days yields 6.3 g. II N(6),5'-diacetate-EtOH, Rf 0.85, m. 113-14.degree., which reacts with 10% aq. AcOH to form I 5'-acetate, Rf 0.23. I 2',3',5'-triacetate, sirup, has Rf 0.67. II (5 g.) and 20 ml. (EtCO)₂O in 125 ml. C₅H₅N yield 5 g. II 5'-propionate, sirup, Rf 0.75, which reacts with 10% aq. AcOH to form I 5'-propionate, m. 170-2.degree. (H₂O and MeOH), Rf 0.44. Other esters prepd. similarly are: I 2',3',5'-tripropionate, sirup, Rf 0.72; II N(6),5'-dibutyrate, sirup, Rf 0.90; I 5'-butyrate, m. 97-8.degree., Rf 0.48; I dibutyrate, sirup; I trilaurate, sirup; I dipalmitate, sirup; I distearate, amorphous powder; I dioleate, sirup; I tribenzoate, m.

100-4.degree.; II 5'-p-nitrobenzoate, powder, Rf 0.80; I 5'-p-nitrobenzoate, Rf 0.30; I tris(p-nitrobenzoate), m. 220.degree. (decompn.); I tris(p-aminobenzoate), amorphous, m. approx. 200.degree.; II 5'-nicotinate, m. 182-3.degree., Rf 0.65; I 5'-nicotinate, m. 157-8.degree., Rf 0.30; I trinicotinate, amorphous, m. approx. 95.degree.; II 5'-isonicotinate, m. 179-81.degree., Rf 0.60; I 5'-isonicotinate, Rf 0.26; I triisonicotinate, Rf 0.70; II 5'-acid succinate, Rf 0.15; I 5'-acid succinate, m. 172-4.degree., Rf 0.40 in 60% aq. PrOH; II 5'-acid phthalate, m. 163-5.degree., Rf 0.15; I bis(acid phthalate), m. 132-4.degree., Rf 0.58. I (5 g.) in C5H5N treated with 4.5 ml. ClSO3H in CHCl3, the product treated with PbO in H2O, the filtered soln. treated with Ag2SO4, refiltered, treated with excess BaCO3, satd. with H2S, filtered, treated with CO2 and concd., and the residue pptd. from H2O with EtOH, yields 12 g. Ba salt of I tris(acid sulfate), Rf 0.22 in 60% aq. PrOH, converted to the Na salt by Na2SO4 or cation exchange resins. Similarly starting with II is prepd. the Ba salt of I 5'-monosulfate, Rf 0.52 in 60% aq. PrOH. I and fuming HNO3 yield a mixt. of I dinitrate, Rf 0.83, and inosine dinitrate, Rf 0.70, m. 190-6.degree. (gas evolution) (aq. dioxane).

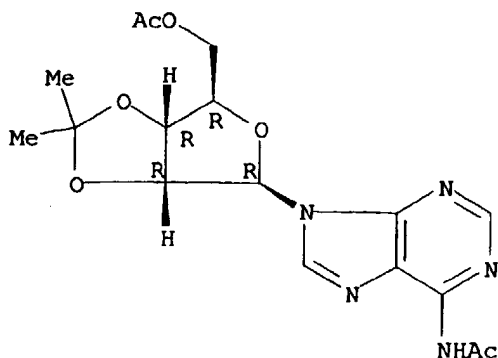
IT 86529-23-9, Adenosine, 2',3'-O-isopropylidene-, 5'-(benzyl phosphorochloridate)
(esters)
RN 86529-23-9 HCAPLUS
CN Adenosine, 2',3'-O-(1-methylethylidene)-, 5'-(phenylmethyl phosphorochloridate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 109816-78-6, Adenosine, N-acetyl-2',3'-O-isopropylidene-, 5'-acetate 113453-89-7, Butyramide, N-[9-(2,3-O-isopropylidene-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, butyrate
(prepn. of)
RN 109816-78-6 HCAPLUS
CN Adenosine, N-acetyl-2',3'-O-isopropylidene-, 5'-acetate (6CI) (CA INDEX NAME)

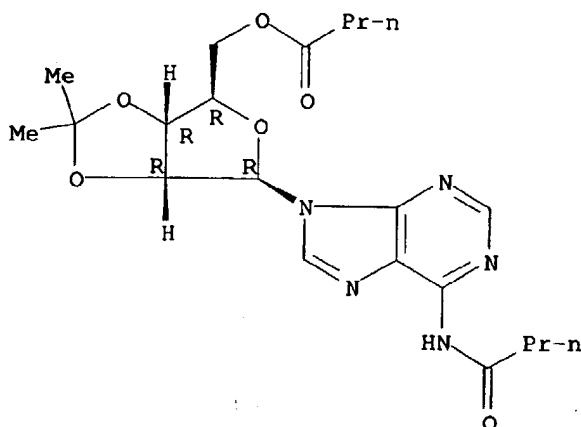
Absolute stereochemistry.



RN 113453-89-7 HCAPLUS

CN Butyramide, N-[9-(2,3-O-isopropylidene-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, butyrate (6CI) (CA INDEX NAME)

Absolute stereochemistry.



L31 ANSWER 1067 OF 1068 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1957:90775 HCAPLUS

DOCUMENT NUMBER: 51:90775

ORIGINAL REFERENCE NO.: 51:16493i,16494a

TITLE: Nucleotides. XLI. Mixed anhydrides as intermediates in the synthesis of dinucleoside phosphates

AUTHOR(S): Hall, R. H.; Todd, Alexander; Webb, R. F.

CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, UK

SOURCE: J. Chem. Soc. (1957) 3291-6

DOCUMENT TYPE: Journal

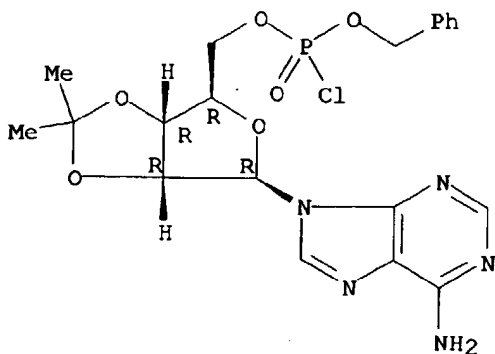
LANGUAGE: Unavailable

AB cf. C.A. 51, 14743i. 5'-Adenosine 5'-uridine phosphate (I) was chosen as a model for an investigation of methods suitable for the synthesis of dinucleoside phosphates. Reactions involving condensation of nucleoside benzyl phosphorochloridates with appropriately protected nucleoside derivs. gave low yields (about 20%). The reaction of the phosphorochloridates with 2,6-lutidine diphenyl phosphate or

trifluoroacetate gave the mixed anhydrides which gave excellent yields (70%) of I. Similar mixed anhydrides of nucleoside phosphites and diphenyl H phosphate were used to prep. the dinucleoside phosphites which were converted via the phosphorochloridate into I.

IT 86529-23-9, Adenosine, 2',3'-O-isopropylidene-, 5'-(benzyl phosphorochloridate)
(and its condensation with nucleosides)
RN 86529-23-9 HCAPLUS
CN Adenosine, 2',3'-O-(1-methylethylidene)-, 5'-(phenylmethyl phosphorochloridate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

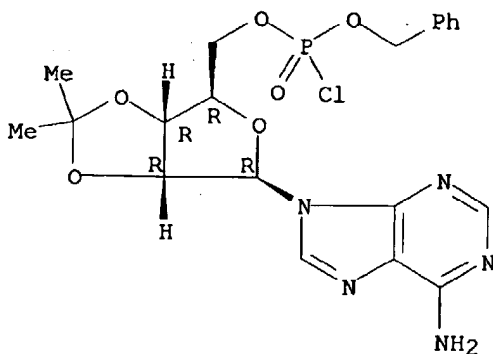


L31 ANSWER 1068 OF 1068 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1957:66670 HCAPLUS
DOCUMENT NUMBER: 51:66670
ORIGINAL REFERENCE NO.: 51:12121b-h
TITLE: Some thionophosphate and phosphoroamidate derivatives of adenosine and certain steroids
AUTHOR(S): Wolff, Manfred E.; Burger, Alfred
CORPORATE SOURCE: Univ. of Virginia, Charlottesville
SOURCE: J. Am. Chem. Soc. (1957), 79, 1970-1
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Et3N (20.2 g.) in 100 cc. dry C6H6 added dropwise with stirring to 38.0 g. Et2NP(O)Cl2 and 18.8 g. PhOH in 300 cc. refluxing dry C6H6 during 45 min., the mixt. refluxed 3 hrs., cooled, and filtered, the filtrate evapd. in vacuo, and the residue treated with 100 cc. dry Et2O, filtered, and fractionated gave 22.5 g. Et2NP(O)- (OPh)Cl (I), b0.4 118.degree., nD25 1.507. The appropriate compd. to be thionophosphorylated (1 equiv.) added with stirring to 1-10 equivs. 3.8% K in dry Me3COH under N, the mixt. dild. with Me3COH at 25.degree. to give a clear soln., the soln. treated dropwise with (EtO)2PSCl as a 30-40% soln. in Me3COH (equiv. to the amt. of K) at 25.degree., refluxed 1-3 hrs. with stirring, and evapd. in vacuo, and the residue dissolved in MeOH or EtOH, filtered, and concd. in vacuo gave the corresponding O,O-di-Et thionophosphate derivs. (II). In this manner were prepd. the following O,O-di-Et thionophosphates (% yield, m.p. or b.p./mm., and optical consts. given): Me 2,3-isopropylidene-5-D-ribofuranosidyl, yellow, 66, 135.degree./0.07 (nD30 1.466), [.alpha.]D30 -46.5.degree. (c 3.81, Me2CO); 3-cholesteryl, plates, 66, 110-11.degree.

(from 95% EtOH) (all m.ps. are cor.), $[\alpha]_D^{23} -31.2^\circ$. (c 2.00, CHCl₃); 3-ergosteryl, 58, 124-5 $^\circ$. (from EtOH-C₆H₆), $[\alpha]_D^{23} -50.0^\circ$. (c 3.30, CHCl₃); 3-estranyl, 46, 78-9 $^\circ$. (from petr. ether and EtOH), $[\alpha]_D^{23} 86.0^\circ$. (c 4.33, CHCl₃).
 2,3'-Isopropylideneadenosine treated similarly with exactly 1 equiv. K, the mixt. kept 0.5 hr. at room temp., adjusted to pH 7 with 5% HCl, and evapd. in vacuo, the residue extd. with MeOH, and the residue from the MeOH ext. triturated with dry Et₂O gave O,O-di-Et O-(2',3'-isopropylidene-5'-adenosyl) thionophosphate (III), hygroscopic, m. 120-30 $^\circ$. [picrate, m. 175-6 $^\circ$. (from 95% EtOH)]. Crude sirupy III from a similar run in 300 cc. 0.1N H₂SO₄ kept 2 days at 27 $^\circ$., neutralized to pH 7 with Ba(OH)₂, and evapd. in vacuo, the powd. residue extd. continually with MeOH, and the ext. concd. in vacuo at 27 $^\circ$. to incipient crystn., heated to boiling, and dild. with petr. ether yielded 37% O,O-di-Et O-(5'-adenosyl) thionophosphate, m. 178-80 $^\circ$. (from EtOH), $[\alpha]_D^{23} -15.1^\circ$. (c 2.15, 5% HCl). 2',3'-Isopropylideneadenosine (6.15 g.), 0.02 mole Me₃COK, and 4.95 g. I gave in the usual manner oily O-Ph O-(2',3'-isopropylidene-5'-adenosyl) phosphorodiethylamidate (IV); picrate monohydrate, yellow, m. 141-3 $^\circ$. (from EtOH). Similarly was prepd. the O-Et analog (V) of IV, glass; picrate hemihydrate, yellow, m. 169-70 $^\circ$. with softening at 160 $^\circ$. (from EtOH). Crude V hydrolyzed with dil. H₂SO₄ in the usual manner gave O-Et O-(5'-adenosyl) phosphorodiethylamidate, glass; yellow picrate, m. 138-40 $^\circ$. with sintering at 125 $^\circ$. (decompn.) (from hot H₂O).

- IT **86529-23-9**, Adenosine, 2',3'-O-isopropylidene-, 5'-(benzyl phosphorochloridate)
 (derivs.)
 RN 86529-23-9 HCAPLUS
 CN Adenosine, 2',3'-O-(1-methylethylidene)-, 5'-(phenylmethyl phosphorochloridate) (9CI) (CA INDEX NAME)

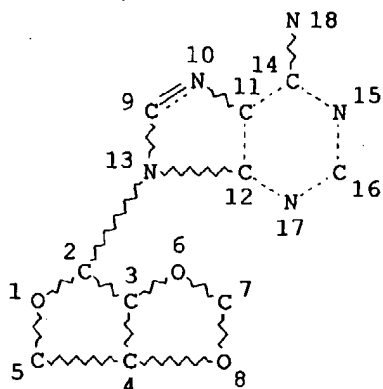
Absolute stereochemistry.



=> d que 110

L1

STR



NODE ATTRIBUTES:

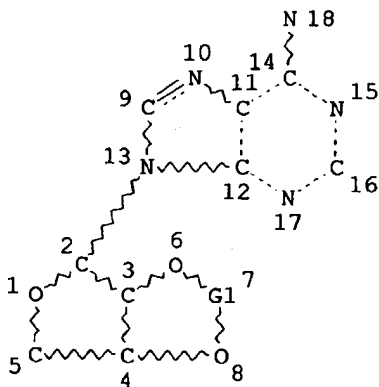
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L2 3214 SEA FILE=REGISTRY SSS FUL L1
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VAR G1=20/23/26

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NSPEC IS RC AT 18
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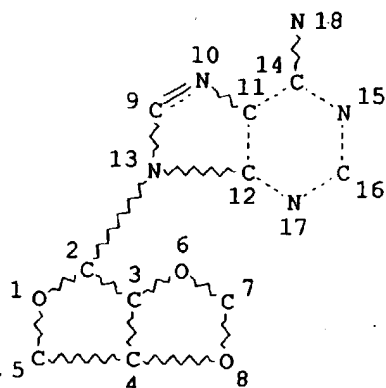
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STEREO ATTRIBUTES: NONE
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April 3, 2003

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NODE ATTRIBUTES:

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DEFAULT MLEVEL IS ATOM

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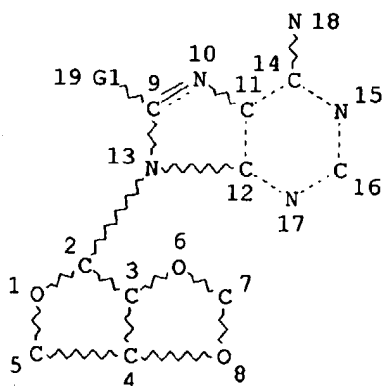
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NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

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L11 STR



VAR G1=F/CL/BR

NODE ATTRIBUTES:

NSPEC IS RC AT 18

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

L12 58 SEA FILE=REGISTRY SUB=L2 SSS FUL L11
 L33 67 SEA FILE=HCAPLUS ABB=ON PLU=ON L12

Only a few
 Refs printed

=> dibib abs hitstr-1-3-45-50-64-67

L33 ANSWER 1 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:284191 HCAPLUS

DOCUMENT NUMBER: 137:79168

TITLE: Oligonucleosides with a nucleobase-including backbone,
 Part 7, syn and anti conformations of a
 (5'-8)-ethynediyl-linked adenosine dimer

AUTHOR(S): Bhardwaj, Punit Kumar; Vasella, Andrea

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Honggerberg,
 HCI, Zurich, CH-8093, Switz.

SOURCE: Helvetica Chimica Acta (2002), 85(3), 699-711

CODEN: HCACAV; ISSN: 0018-019X

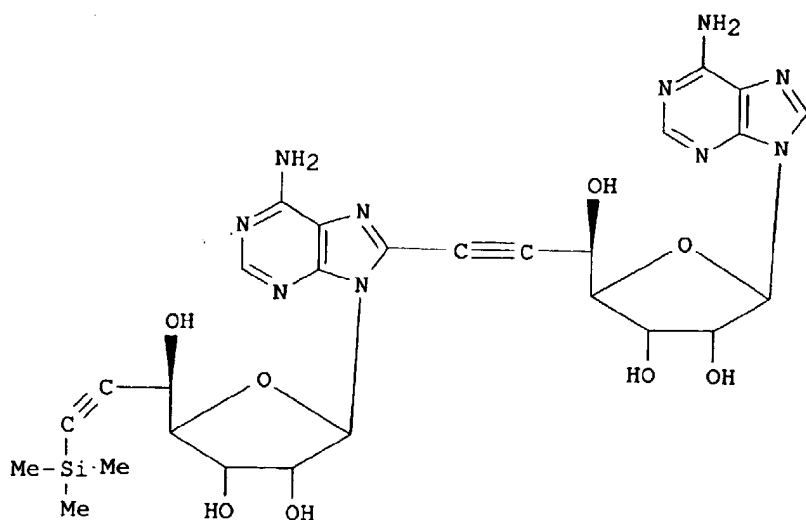
PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:79168

GI

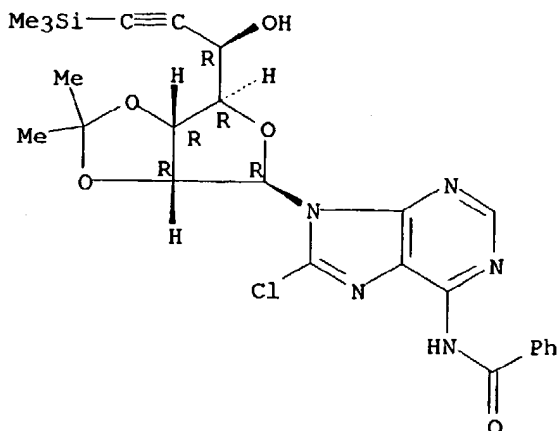


I

AB The conformational anal. of (I) was carried out in (D6)DMSO and in mixts. of (D6)DMSO and CDCl₃ to evaluate the syn/anti conformations, relevant to the pairing propensity of this type of nucleotide analog. The HO-C(5') of (right) unit a and of (left) unit b of I form an intramol. H-bond to N(3). In (D6)DMSO, the C(5')-OH...N(3) H-bond in unit a is partially broken, while that in unit b persists to a larger extent. The syn conformation prevails for unit a and particularly for unit b. The furanosyl moieties adopt predominantly a 2'-endo conformation that is largely independent of

the solvent.
 IT 292642-48-9
 RL: MSC (Miscellaneous)
 (model compds. for the conformational anal. of (5'-8)-ethynediyl-linked adenosine dimer and the effects of intramol. hydrogen bonds)
 RN 292642-48-9 HCAPLUS
 CN Benzamide, N-[8-chloro-9-[6,7-dideoxy-2,3-O-(1-methylethylidene)-7-(trimethylsilyl)-.beta.-D-allo-hept-6-ynofuranosyl]-9H-purin-6-yl]- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

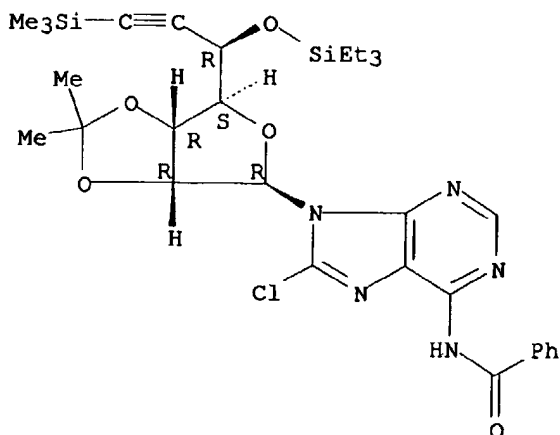


REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 2 OF 67 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 2001:48526 HCAPLUS
 DOCUMENT NUMBER: 134:208043
 TITLE: Oligonucleosides with a nucleobase-including backbone-part 4: a convergent synthesis of ethynediyl-linked adenosine tetramers
 AUTHOR(S): Gunji, Hiroki; Vasella, Andrea
 CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.
 SOURCE: Helvetica Chimica Acta (2000), 83(12), 3229-3245
 CODEN: HCACAV; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:208043
 AB Ethynediyl-linked adenosine tetramer oligoribonucleosides were prepd. via iodination, 1,3-dipolar cycloaddn., and coupling of iodinated dimer with alkyne nucleosides. There is no UV evidence for a base-base interaction in the protected and deprotected dimers and tetramers.
 IT 292642-52-5 292642-53-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of ethynediyl-linked adenosine tetramer oligonucleosides via iodination, 1,3-dipolar cycloaddn., and coupling reactions)
 RN 292642-52-5 HCAPLUS

CN Benzamide, N-[8-chloro-9-[6,7-dideoxy-2,3-O-(1-methylethylidene)-5-O-(triethylsilyl)-7-(trimethylsilyl)-.beta.-D-allo-hept-6-ynofuranosyl]-9H-purin-6-yl]- (9CI) (CA INDEX NAME)

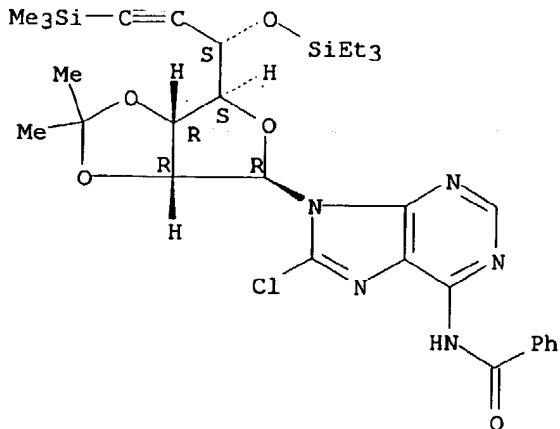
Absolute stereochemistry. Rotation (+).



RN 292642-53-6 HCAPLUS

CN Benzamide, N-[8-chloro-9-[6,7-dideoxy-2,3-O-(1-methylethylidene)-5-O-(triethylsilyl)-7-(trimethylsilyl)-.alpha.-L-talo-hept-6-ynofuranosyl]-9H-purin-6-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 328241-11-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

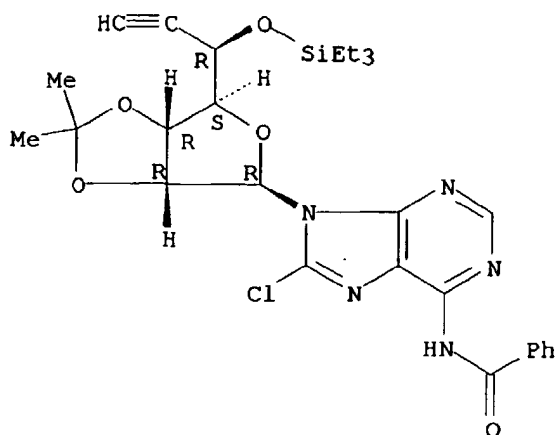
(prepn. of ethynediyl-linked adenosine tetramer oligonucleosides via iodination, 1,3-dipolar cycloaddn., and coupling reactions)

RN 328241-11-8 HCAPLUS

CN Benzamide, N-[8-chloro-9-[6,7-dideoxy-2,3-O-(1-methylethylidene)-5-O-(triethylsilyl)-.beta.-D-allo-hept-6-ynofuranosyl]-9H-purin-6-yl]- (9CI)

(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 3 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:502875 HCAPLUS

DOCUMENT NUMBER: 133:238228

TITLE: Oligonucleosides with a nucleobase-including backbone part 2 synthesis and structure determination of adenosine-derived monomers

AUTHOR(S): Gunji, Hiroki; Vasella, Andrea

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (2000), 83(7), 1331-1345

CODEN: HCACAV; ISSN: 0018-019X

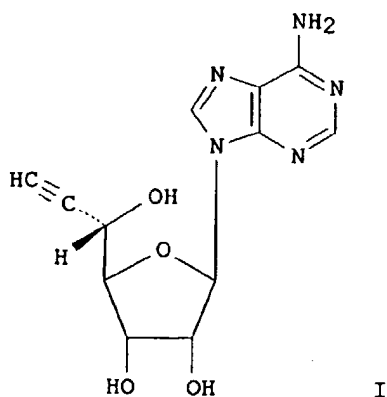
PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

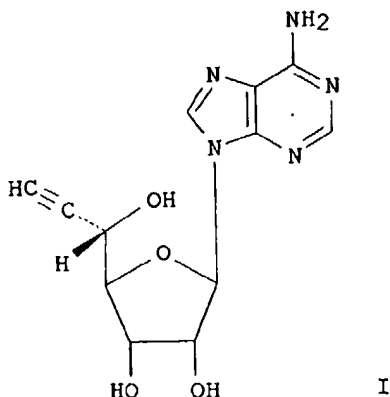
LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:238228

GI



I



AB The synthesis and structure detn. of adenosine-derived monomeric, e.g. I, building blocks for new oligonucleotides via addn. of propargylic silyl ethers with partially protected adenosine, are described.

IT 292642-44-5P 292642-45-6P 292642-48-9P

292642-49-0P 292642-52-5P 292642-53-6P

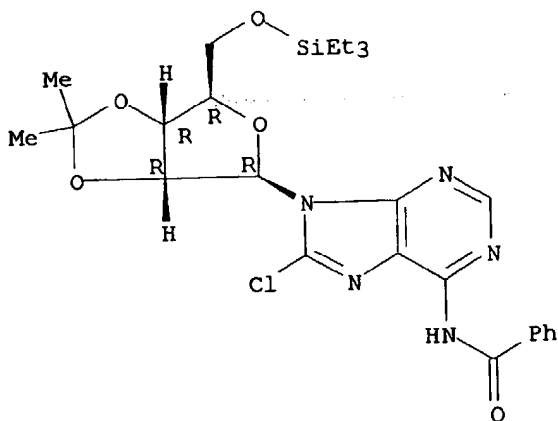
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and structure detn. of adenosine-derived monomers via addn. of propargylic silyl ethers with partially protected adenosines)

RN 292642-44-5 HCAPLUS

CN Adenosine, N-benzoyl-8-chloro-2',3'-O-(1-methylethylidene)-5'-O-(triethylsilyl)- (9CI) (CA INDEX NAME)

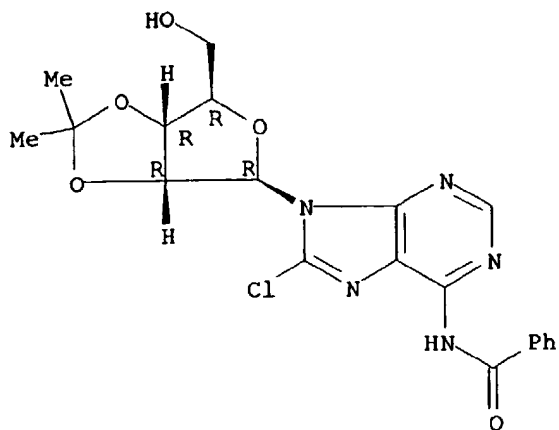
Absolute stereochemistry. Rotation (-).



RN 292642-45-6 HCAPLUS

CN Adenosine, N-benzoyl-8-chloro-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

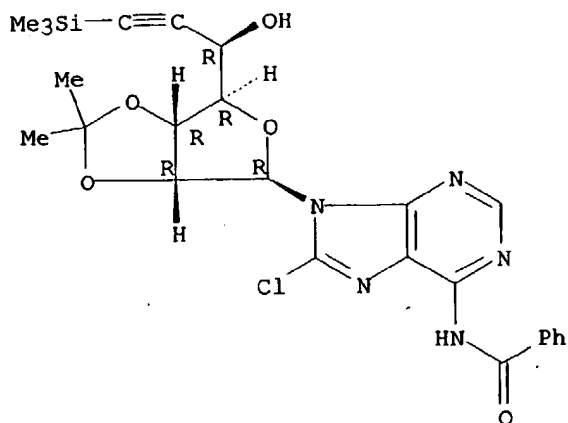
Absolute stereochemistry. Rotation (-).



RN 292642-48-9 HCAPLUS

CN Benzamide, N-[8-chloro-9-[6,7-dideoxy-2,3-O-(1-methylethylidene)-7-(trimethylsilyl)-.beta.-D-allo-hept-6-ynofuranosyl]-9H-purin-6-yl]- (9CI)
(CA INDEX NAME)

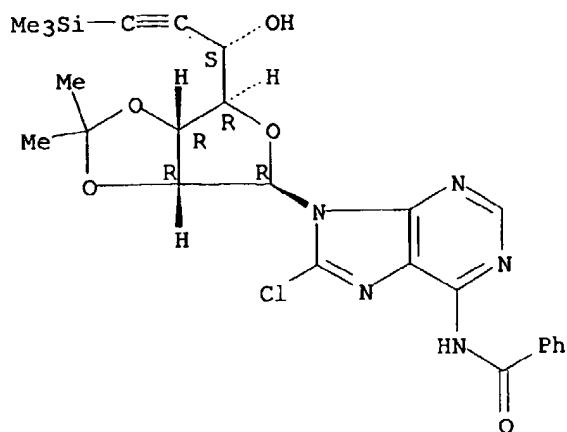
Absolute stereochemistry. Rotation (-).



RN 292642-49-0 HCAPLUS

CN Benzamide, N-[8-chloro-9-[6,7-dideoxy-2,3-O-(1-methylethylidene)-7-(trimethylsilyl)-.alpha.-L-talo-hept-6-ynofuranosyl]-9H-purin-6-yl]- (9CI)
(CA INDEX NAME)

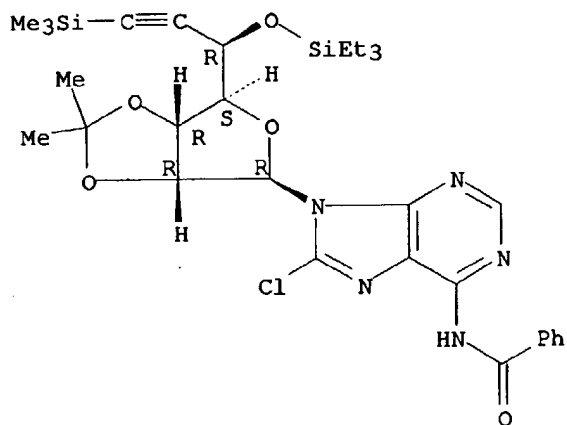
Absolute stereochemistry. Rotation (+).



RN 292642-52-5 HCAPLUS

CN Benzamide, N-[8-chloro-9-[6,7-dideoxy-2,3-O-(1-methylethylidene)-5-O-(triethylsilyl)-7-(trimethylsilyl)-.beta.-D-allo-hept-6-ynofuranosyl]-9H-purin-6-yl]- (9CI) (CA INDEX NAME)

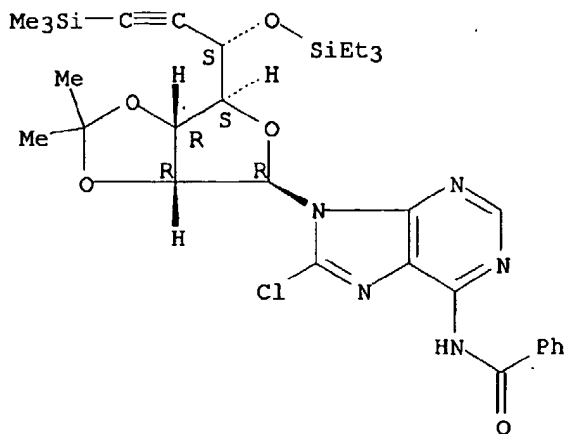
Absolute stereochemistry. Rotation (+).



RN 292642-53-6 HCAPLUS

CN Benzamide, N-[8-chloro-9-[6,7-dideoxy-2,3-O-(1-methylethylidene)-5-O-(triethylsilyl)-7-(trimethylsilyl)-.alpha.-L-talo-hept-6-ynofuranosyl]-9H-purin-6-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 45 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1979:439769 HCAPLUS

DOCUMENT NUMBER: 91:39769

TITLE: Nucleosides and nucleotides. XXVII. Synthesis of 2- and 8-cyanoadenosines and their derivatives

AUTHOR(S): Matsuda, Akira; Nomoto, Yuji; Ueda, Tohru
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1979), 27(1), 183-92

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A facile displacement of a methylsulfonyl group in adenosines with cyanide ion is described. Treatment of protected 8-(methylsulfonyl)adenosines with NaCN in DMF gave the 8-cyanoadenosine. The conversion of the cyano group to the Me imidate, methoxycarbonyl, carbamoyl, and carboxylic acid was achieved. Similar reaction was carried out with 2-(methylsulfonyl)adenosine to give the 2-cyanoadenosine and their derivs. The NMR and CD spectra of these 2- and 8-substituted adenosines are given. The 8-substituted adenosines possess syn-conformations while the 2-substituted derivs. prefer anti-conformations, as confirmed by the CD and NMR spectra.

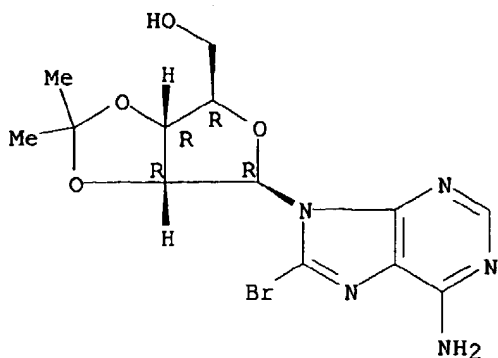
IT 13089-45-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(methylthiolation of)

RN 13089-45-7 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 46 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1979:168903 HCAPLUS

DOCUMENT NUMBER: 90:168903

TITLE: Photochemical cyclization of 2',3'-O-isopropylidene-8-phenylthioadenosine to the 8,5'(R)- and 8,5'(S)-cycloadenosines (nucleosides and nucleotides - XVIII)

AUTHOR(S): Matsuda, A.; Tezuka, M.; Ueda, T.

CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, Japan

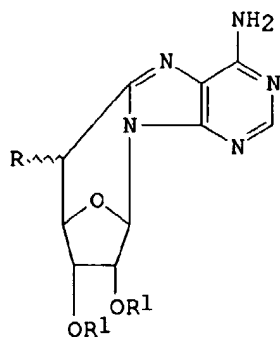
SOURCE: Tetrahedron (1978), 34(16), 2449-52

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB 2',3'-O-isopropylidene-8-phenylthioadenosine, prepd. (85.3%) by reaction of 2',3'-O-isopropylidene-8-bromoadenosine with NaSPh in abs. MeOH (60.degree., room temp., overnight), cyclized to cycloadenosines I (R = .alpha.-, .beta.-OH, R12 = CMe2) on irradiation (MeCN, Me3COOH, 4 h). Deacetonation (HCl, 85-90.degree., 1 h) of the latter derivs. gave I (R = .alpha.-, .beta.-OH, R1 = H).

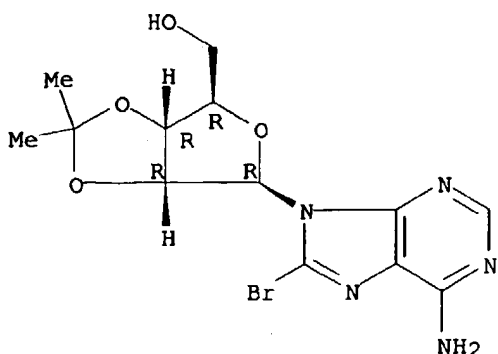
IT 13089-45-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(thiophenoxylation of)

RN 13089-45-7 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 47 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1979:121924 HCAPLUS

DOCUMENT NUMBER: 90:121924

TITLE: Studies on nucleosides and nucleotides. LXXXI.
Carbon-13 magnetic resonance spectra of 8-substituted
purine nucleotides. Effects of various phosphate
groups on the chemical shifts and conformation of
nucleotides

AUTHOR(S): Uesugi, Seiichi; Ikehara, Morio

CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1978), 26(10),
3040-9

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 13C-NMR spectra of 8-substituted purine nucleotides including the 2'-, 3'-, 2',3'-cyclic, 5'- and 3',5'-cyclic phosphates of 8-bromoadenosine and the 5'phosphates of 8-bromoguanosine, 8-methylinosine and 2-methylthio-8-methylinosine. All the 8-substituted nucleotides showed a characteristic upfield shift (-0.9 to -3.7 ppm) of the 2'-C with respect to the corresponding parent nucleotides. These results show that they take a syn conformation in aq. soln. to some extent. It was concluded from consideration of the sugar puckerings in the published PMR data that the 5'-phosphate of 8-bromoadenosine takes a more rigid syn conformation than the 2'-, 3'- and 2', 3'-cyclic phosphates. It is also suggested that 8-bromoadenosine has a flexible glycosidic conformation similar to those for the latter compds. in water while in Me2SO it adopts a more rigid conformation. The 5'-phosphates of the other 8-substituted nucleosides were also assumed to adopt a rigid syn conformation. The influences of various types of phosphate groups on the C chem. shifts are also discussed. Relatively large upfield shifts were obsd. for the C(4') signal of the 8-substituted 5'-nucleotides which has been assumed to be a reflection of a high population of non-gg conformations about the C(4')-C(5') bond.

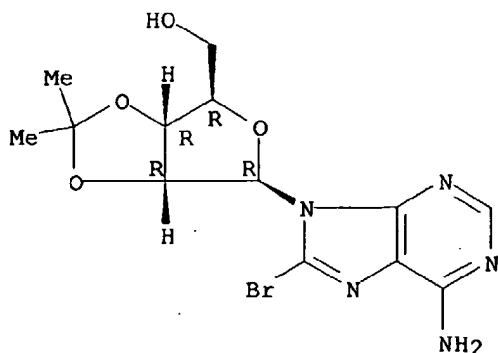
IT 13089-45-7

RL: PRP (Properties)
(carbon-13 NMR of)

RN 13089-45-7 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 48 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1978:597854 HCAPLUS

DOCUMENT NUMBER: 89:197854

TITLE: Conformational analysis of 2',3'-O-isopropylidene adenosine derivatives by proton NMR

AUTHOR(S): Gaudemer, Alain; Nief, Francois; Pontikis, Renee; Zylber, Jean

CORPORATE SOURCE: Lab. Chim. Coord. Bioorg., Univ. Paris Sud, Orsay, Fr.

SOURCE: Organic Magnetic Resonance (1977), 10, 135-45

CODEN: ORMRBD; ISSN: 0030-4921

DOCUMENT TYPE: Journal

LANGUAGE: French

AB Conformational anal. using ¹H NMR is reported for 36 derivs. of 2',3'-O-isopropylideneadenosine with substituents at C-5', C-8, and N-6. Conformational modifications were assigned to specific interactions between the sugar and purine moieties and to solvent effects.

IT 13089-45-7 20789-78-0

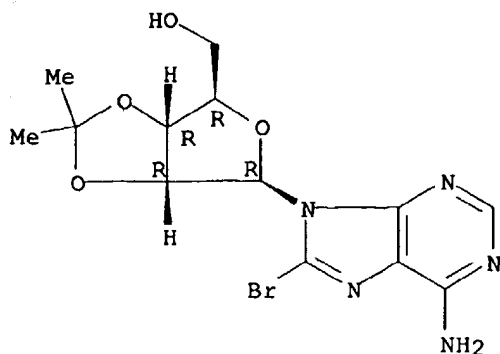
RL: PRP (Properties)

(conformation of, NMR study of)

RN 13089-45-7 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

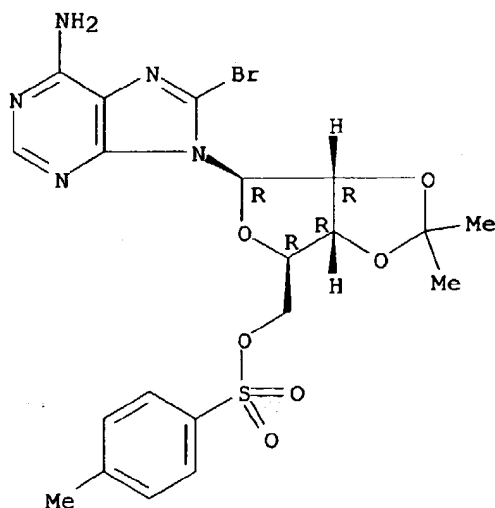
Absolute stereochemistry.



RN 20789-78-0 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)-, 5'-(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 49 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1978:424683 HCAPLUS

DOCUMENT NUMBER: 89:24683

TITLE: Convenient synthesis of some purine 8,5'-imino cyclonucleosides

AUTHOR(S): Sasaki, Tadashi; Minamoto, Katsumaro; Itoh, Hidemi

CORPORATE SOURCE: Fac. Eng., Nagoya Univ., Nagoya, Japan

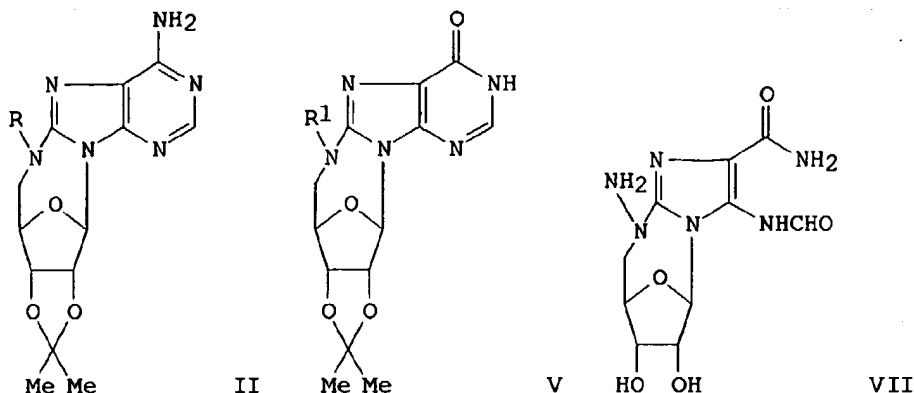
SOURCE: Journal of Organic Chemistry (1978), 43(12), 2320-5

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Purine 8,5'-imino and aminimino cyclonucleosides were prep'd. from 2',3'-O-isopropylidene-5'-O-tosyl-8-bromoadenosine (I) and anhyd. hydrazine. Treating I with anhyd. hydrazine in EtOH gave 8,5'-aminiminoadenine II (R = NH₂) (III), which was oxidized to the corresponding 8,5'-imino cyclonucleoside II (R = H) (IV). The N-amino group in III was quant. protected with hot AcOH and phthalic anhydride to give II (R = AcNH, phthalimido). Acidic treatment of III and IV gave the deblocked parent cyclonucleosides, whereas treating II (R = NH₂, AcNH, phthalimido) with nitrous acid gave inosine analogs, e.g. V (R₁ = phthalimido) (VI). Dephthaloylation of VI with NH₂NH₂-MeOH gave V (R₁ = NH₂) as a 1:1 complex with the released phthalazine-1,4-dione, which was deblocked with 90% CF₃CO₂H. Treating V (R₁ = NH₂) or its deblocked analog with MeOH-concd. HCl (3:1) gave VII.

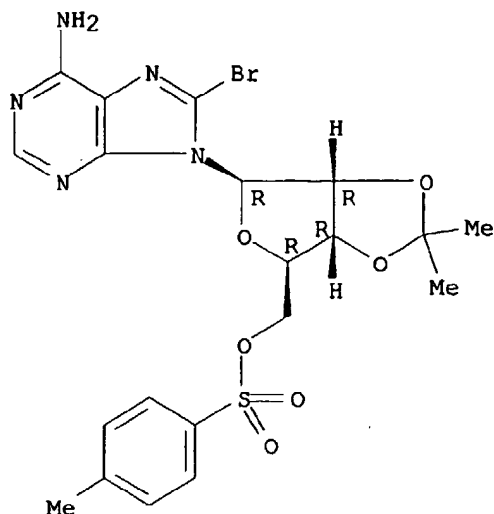
IT 20789-78-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydrazine)

RN 20789-78-0 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)-, 5'-(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 50 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1977:90174 HCAPLUS

DOCUMENT NUMBER: 86:90174

TITLE: Synthesis of 8-carbamoyl- and 8-carboxyadenosine 3',5'-cyclic phosphates

AUTHOR(S): Naka, Takehiko; Honjo, Mikio

CORPORATE SOURCE: Cent. Res. Div., Takeda Chem. Ind., Ltd., Osaka, Japan

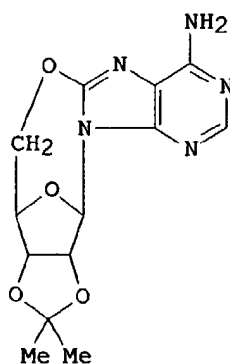
SOURCE: Chemical & Pharmaceutical Bulletin (1976), 24(9), 2052-6

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



III

AB Reaction of 8-bromo-cAMP (cAMP = adenosine 3',5'-cyclic phosphate) (I) with KCN in hot DMF gave 8-carbamoyl-cAMP (II). II was hydrolyzed with aq. NaOH to 8-carboxy-cAMP, which was converted to cAMP by heating in Me₂SO. A similar reaction of 8-bromo-5'-AMP or 8-bromo-2',3'-O-

isopropylideneadenosine with KCN in DMF yielded 8-bromoadenosine or 8,5'-anhydro-2',3'-O-isopropylidene-8-hydroxyadenosine (III), resp. Treatment of 5'-nucleotides with hot aq. DMF afforded the corresponding nucleosides.

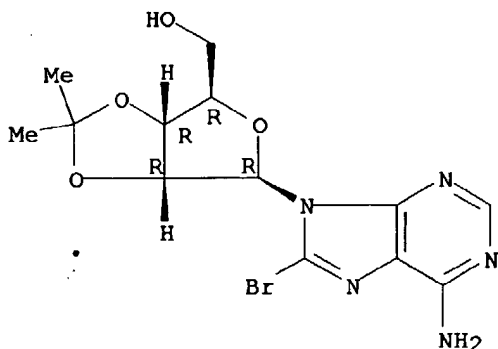
IT 13089-45-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

RN 13089-45-7 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 64 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1967:403214 HCAPLUS

DOCUMENT NUMBER: 67:3214

TITLE: Studies of nucleosides and nucleotides. XXXII.
Purine cyclonucleosides. 3. Synthesis of 2'-deoxy-
and 3'-deoxyadenosine from adenosine

AUTHOR(S): Ikehara, Morio; Tada, Hiroshi

CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Hokkaido, Hokkaido, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1967), 15(1),
94-100

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 63: 2030b; 64: 17700e. A mixt. of 2 g. 2',3'-O-isopropylideneadenosine and 2.2 g. N-bromoacetamide in 20 ml. dry CHCl₃ was refluxed 5 hrs., the solvent was removed, and the residue was taken up in 50 ml. EtOAc, washed with 10% NaHSO₄, NaHCO₃, and water, dried, and distd. to give 1.2 g. 8-bromo-2',3'-O-isopropylideneadenosine (I), m. 215-17.degree. (EtOH). I (1.38 g.) was acetylated with 6 ml. Ac₂O in 35 ml. pyridine at room temp. overnight, 20 ml. EtOH was added, and the mixt. was kept at room temp. 2 hrs. to give 1.01 g. 5'-O-acetyl-8-bromo-2',3'-O-isopropylideneadenosine (II), m. 158-60.degree. (EtOH). A mixt. of 4 g. 5'-O-acetyl-2',3'-O-isopropylideneadenosine and 5 g. N-bromoacetamide in 50 ml. CHCl₃ was refluxed 6 hrs. and worked up as above to give 3 g. II, m. 155-6.degree. (EtOH). A soln. of 1 g. II in 30 ml. 98% HCO₂H was kept at room temp. 20 hrs. under dry conditions, 20 ml. EtOH was added, and the solvent was distd. in vacuo to give 600 mg. 5'-O-acetyl-8-bromoadenosine (III). III (998 mg.) was dried by azeotropic distn. with dry pyridine,

and then in 60 ml. dry pyridine, 499 mg. p-MeC₆H₄SO₂Cl was added with ice cooling, and the stoppered mixt. was refrigerated 60 hrs., worked up dissolved in 20 ml. MeOH satd. with NH₃ at 0.degree., and refrigerated for 21 hrs. to give 155 mg. 8-bromo-2'-O-p-tolylsulfonyl-adenosine (IV), m. 220-3.degree. (decomp.) (50% iso-PrOH). The residue from the mother liquor was recrystd. from 50% iso-PrOH to give a p-tolylsulfonylated mixt. contg. needles, m. 176-7.degree. and granulous crystals, m. 213.degree. (decomp.). A mixt. of 510 mg. IV in 60 ml. BuOH was refluxed with 81.5 mg. thiourea 2 hrs., the solvent was evapd. in vacuo, and the residue in 10 ml. EtOH was chromatographed on 70 g. cellulose powder and eluted with 100 parts BuOH satd. with water and 1 part concd. NH₃. Fractions of 10 ml. each were collected. Fractions 11-18 were evapd. to give 167 mg. 8,2'-anhydro-9-.beta.-D-arabinofuranosyl-8-mercaptoadenine (V), m. 191-4.degree. (water), [.alpha.]_D^{23.5} -187.2.degree. (c 1.0, H₂O). The p-tolylsulfonylated mixt. above (1.67 g.) was refluxed with 277 mg. thiourea in 100 ml. BuOH 2 hrs., the solvent was evapd. in vacuo, and the residue in 10 ml. EtOH was chromatographed on 120 g. cellulose powder and eluted as above. Fractions 12-23 were evapd. to give 8,2'-anhydro-8-mercapto-(3-O-p-tolylsulfonyl-9-.beta.-D-arabinofuranosyl)adenine (VI), m. 196-7.degree. (2:1 EtOH-water), [.alpha.]_D²³ -70.8.degree. (c 0.5, pyridine). Fractions 28-30 were evapd. to give 8,3'-anhydro-8-mercapto-9-.beta.-D-xylofuranosyladenine (VII), colors at 231-2.degree., decompd. at 250.degree.. Fractions 31-4 gave 110 mg. V and a minor component presumably 8-mercapto-2'(or 3')-O-p-tolylsulfonyl-adenosine. V (210 mg.) was refluxed in 20 ml. water with 1.5 g. Raney Ni 6 hrs., the mixt. was filtered, and the filtrate and washings were evapd. in vacuo to give 2'-deoxyadenosine, m. 187-8.degree.. VII (10 mg.) was refluxed in 10 ml. H₂O with Raney Ni for 1 hr. to give 3'-deoxyadenosine (cordycepin). VI (67 mg.) was refluxed in 14 ml. PrOH and 7 ml. water with 500 mg. Raney Ni for 5.5 hrs., the mixt. was filtered, and the filtrate was evapd. in vacuo to give 3'-O-p-tolylsulfonyl-2'-deoxyadenosine, m. 156-70.degree..

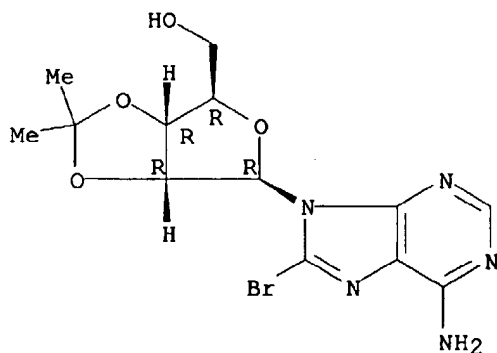
IT 13089-45-7P 13089-46-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 13089-45-7 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

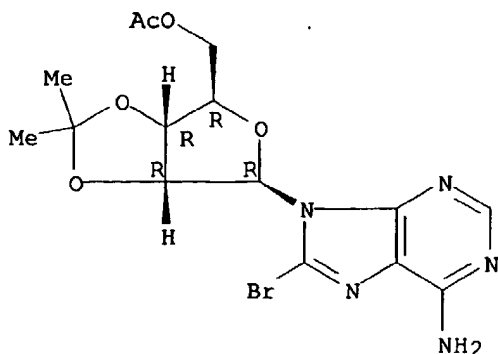
Absolute stereochemistry.



RN 13089-46-8 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-isopropylidene-, 5'-acetate (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 65 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1967:85984 HCAPLUS

DOCUMENT NUMBER: 66:85984

TITLE: Bromination of adenosine nucleosides and nucleotides.

AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi; Kaneko, Masakatsu

CORPORATE SOURCE: Hokkaido Univ., Sapporo, Japan

SOURCE: Chemical Communications (London) (1967), (1), 17-18

CODEN: CCOMA8; ISSN: 0009-241X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A soln. of di-Na adenosine 5'-monophosphate in 0.1N NaOH treated very slowly with 1 mole Br in H₂O at room temp., the mixt. kept 7 hrs., adsorbed on a Dowex 1 column (HCO₂⁻ form), and eluted with 0.1N HCO₂H gave 81% di-Na 8-bromoadenosine 5'-monophosphate. Under similar conditions 100% 8-bromoadenine and 66% 8-bromo-2'-deoxyadenine were obtained from, resp., adenine and 2'-deoxyadenine. 2',3'-O-Isopropylideneadenosine (1 millimole) dissolved in 15 ml. dioxane and 15 ml. 10% Na₂HPO₄, treated with 1.5 equiv. Br, the mixt. agitated 5 hrs. at room temp., kept overnight, and extd. with CHCl₃ gave 80% 8-bromo-2',3'-O-isopropylideneadenosine, m. 224-5.degree..

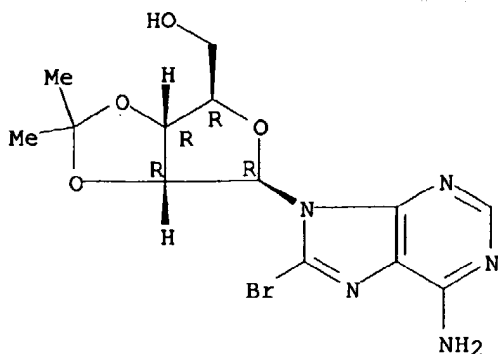
IT 13089-45-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 13089-45-7 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 66 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1966:465763 HCAPLUS

DOCUMENT NUMBER: 65:65763

ORIGINAL REFERENCE NO.: 65:12275g-h,12276a

TITLE: Synthesis of purine cyclonucleoside having an 8,2'-O-anhydro linkage

AUTHOR(S): Ikehara, Morio; Tada, Hiroshi; Muneyama, Kei; Kaneko, Masakatsu

CORPORATE SOURCE: Hokkaido Univ., Sapporo, Japan

SOURCE: J. Am. Chem. Soc. (1966), 88(13), 3165-7

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The synthesis of the 1st purine cydonucleoside I having an O-anhydro linkage was reported (CA 62, 13220d). The prepn. involved bromination of 2',3'-O-isopropylideneadenosine to its 8-bromo deriv. (II), acetylation of II to 5'-O-acetyl-8-bromo-2',3'-O-isopropylideneadenosine (III), hydrolysis of III with HCO₂H to 5'-O-acetyl-8-bromoadenosine (IV), and p-toluenesulfonation of IV followed by deacetylation, debromination, and desulfonation (use of BzONa in HCONMe₂ 2 hrs. at 100-5.degree.) to give I, [.alpha.]_D¹⁹ -121.6.degree. (c 0.75, pyridine), which was purified by column chromatography on cellulose. Refluxing I 2 hrs. in 0.1N H₂SO₄ afforded 9-glycosyl-8-hydroxyadenine and 8-hydroxyadenine, and I treated with BzONa in HCONMe₂ in the presence of BzOH gave 9-(2-O benzoyl-.beta.-D-ribofuranosyl)-8-hydroxyadenine.

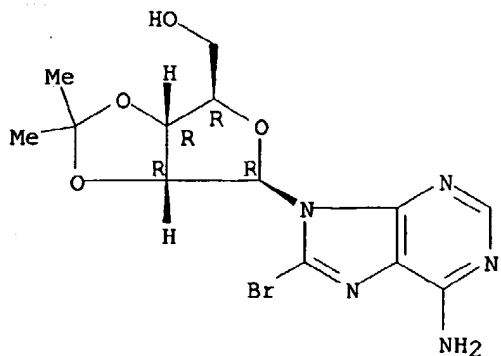
IT 13089-45-7, Adenosine, 8-bromo-2',3'-O-isopropylidene-

13089-46-8, Adenosine, 8-bromo-2',3'-O-isopropylidene-, 5'-acetate (prepn. of)

RN 13089-45-7 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

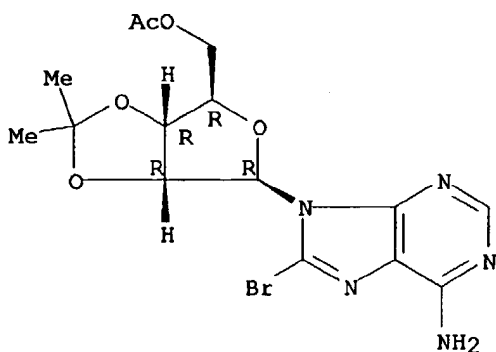
Absolute stereochemistry.



RN 13089-46-8 HCAPLUS

CN Adenosine, 8-bromo-2',3'-O-isopropylidene-, 5'-acetate (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 67 OF 67 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1962:60818 HCAPLUS

DOCUMENT NUMBER: 56:60818

ORIGINAL REFERENCE NO.: 56:11692d-g

TITLE: Nucleosides and nucleotides. VI. Synthesis of 9-(5'-deoxy-5'-iodo-β-D-ribofuranosyl)-2,8-dichloroadenine

AUTHOR(S): Kanazawa, Teiichi

CORPORATE SOURCE: Tokyo Inst. Technol.

SOURCE: Nippon Kagaku Zasshi (1960), 81, 1299-302

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB 9-(2',3'-O-Isopropylidene-β-D-ribofuranosyl)-2,8-dichloroadenine (I) (1.45 g.), prepd. by acetylating of 2,8-dichloroadenosine, kept with p-toluenesulfonyl chloride in pyridine 1 day gave 1.3 g. 9-(2,3-O-isopropylidene-5-O-p-tolylsulfonyl-β-D-ribofuranosyl)-2,8-dichloroadenine (II) (amorphous). II (1.3 g.) heated with NaI in Me₂CO in a sealed tube 1.5 hrs. gave 0.77 g. 9-(2,3-O-isopropylidene-5-deoxy-5-iodo-β-D-ribofuranosyl)-2,8-dichloroadenine (III), m. 172.degree. [α]_D²⁵ -23.1.degree. (c 2.25, dioxane), λ_{max} 267 mμ.,

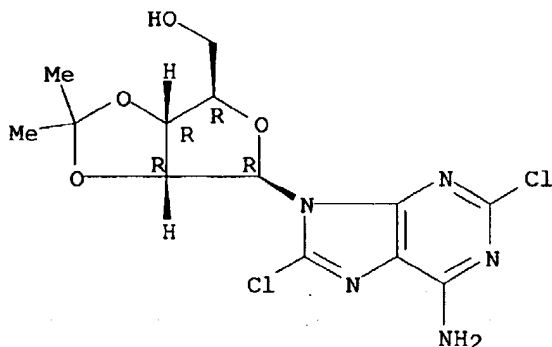
.epsilon. 12,200. III hydrolyzed with HNO₃ in dioxane 32 hrs. at 10.degree. thereafter 8 hrs. at 20.degree. gave 85% 9-(5-deoxy-5-iodo-.beta.-D-ribofuranosyl)-2,8-dichloroadenine (IV), m. 175.degree. (decompn.). An EtOH soln. of 13.5 g. HgCl₂ was added to a 0.1N NaOH soln. of 10.2 g. 2,8-dichloroadenine (V) contg. Celite, and resulting V HgCl₂ salt (VI) with Celite carrier was filtered off and washed. VI treated with 2,3-di-O-acetyl-5-deoxy-5-iodo-D-ribofuranosyl chloride (VII), prepd. from 7.7 g. 1,2,3-tri-O-acetyl-5-deoxy-5-iodo-.beta.-D-ribofuranose (VIII), gave 10 g. 9-(2,3-O-acetyl-5-deoxy-5-iodo-.beta.-D-ribofuranosyl)-2,8-dichloroadenine (IX), m. 183-5.degree.. V (1 g.) reduced with NH₃ 24 hrs. at 0.degree. in MeOH gave 0.8 g. IV. VII, prepd. from 5 g. VIII, boiled with 8.8 g. VI in xylene and the resulting sirup chromatographed gave 0.8 g. IX and 0.15 g. [2,3-di-O-acetyl-5-deoxy-5-(2,8-dichloroadenyl)-D-ribofuranosyl]-2,8-dichloroadenine (X).

IT 96535-65-8, Adenosine, 2,8-dichloro-2',3'-O-isopropylidene-
96984-02-0, Adenosine, 2,8-dichloro-5'-deoxy-5'-iodo-2',3'-O-isopropylidene- 100000-46-2, Adenosine, 2,8-dichloro-2',3'-O-isopropylidene-, 5'-p-toluenesulfonate
(prepn. of)

RN 96535-65-8 HCAPLUS

CN Adenosine, 2,8-dichloro-2',3'-O-isopropylidene- (7CI) (CA INDEX NAME)

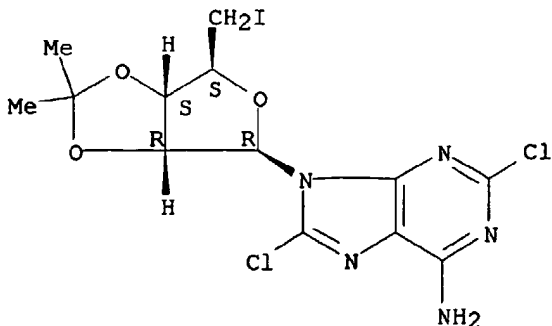
Absolute stereochemistry.

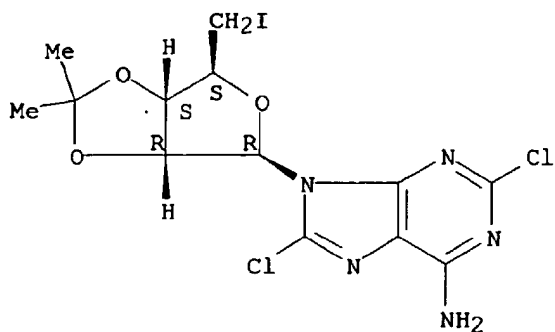


RN 96984-02-0 HCAPLUS

CN Adenosine, 2,8-dichloro-5'-deoxy-5'-iodo-2',3'-O-isopropylidene- (7CI)
(CA INDEX NAME)

Absolute stereochemistry.

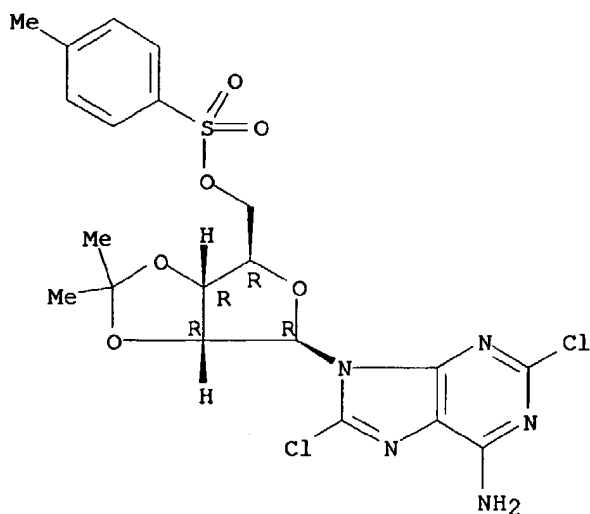




RN 100000-46-2 HCAPLUS

CN Adenosine, 2,8-dichloro-2',3'-O-isopropylidene-, 5'-p-toluenesulfonate
(7CI) (CA INDEX NAME)

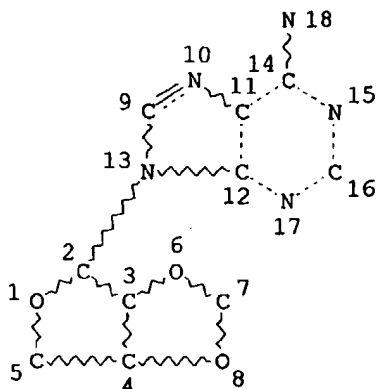
Absolute stereochemistry.



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L1

STR



NODE ATTRIBUTES:

NSPEC IS RC AT 18

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

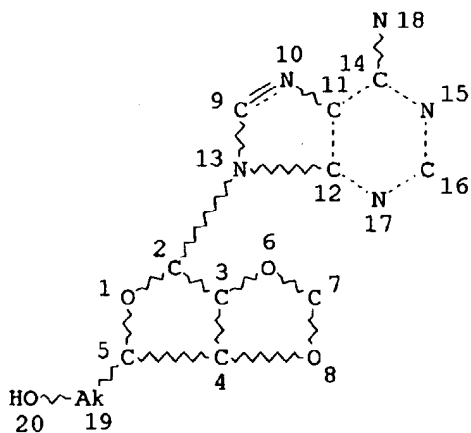
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L2 3214 SEA FILE=REGISTRY SSS FUL L1

L14

STR



NODE ATTRIBUTES:

NSPEC IS RC AT 18

CONNECT IS E3 RC AT 5

CONNECT IS E2 RC AT 19

DEFAULT MLEVEL IS ATOM

GGCAT IS LOC AT 19

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L15 556 SEA FILE=REGISTRY SUB=L2 SSS FUL L14
~~L34~~ 824 SEA FILE=HCAPLUS ABB=ON PLU=ON L15

only a few
Refs printed.

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L34 ANSWER 1 OF 824 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:831353 HCAPLUS
DOCUMENT NUMBER: 138:73419
TITLE: Gel formation properties of a uracil-appended
cholesterol gelator and cooperative effects of the
complementary nucleobases
AUTHOR(S): Snip, Erwin; Koumoto, Kazuya; Shinkai, Seiji
CORPORATE SOURCE: Chemotransfiguration Project, Japan Science and
Technology Corporation (JST), Kurume, Fukuoka,
839-0861, Japan
SOURCE: Tetrahedron (2002), 58(43), 8863-8873
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

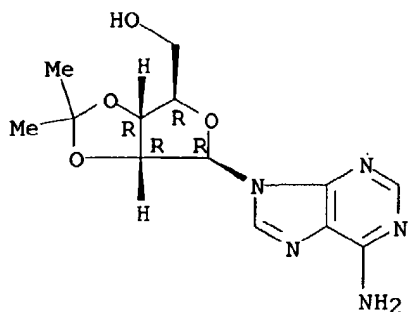
- AB The authors designed and synthesized a uracil-appended cholesterol gelator I in order to control the gel stability and the gel morphol. by addn. of the complementary and non-complementary nucleobase derivs. Compd. I forms columnar stacks in cyclohexane due to the van der Waals interaction (cholesterol-cholesterol interaction) and the intergelator hydrogen bonding between uracil moieties. Addn. of a 'monomeric' adenosine, II, into the gel only decreases the stability with increasing the concn. The destabilization is ascribed to a lack of intergelator hydrogen bonding accompanied with forming the complementary base pairs between I and II. In contrast, addn. of an adenine-appended cholesterol induces a different behavior; with increasing concn. the mixed gel is initially stabilized and then destabilized, giving rise to a max. at the ratio of I/adenine-appended cholesterol = 1:1 for the Tgel plot. One may consider, therefore, that when the additive has a common, column-forming cholesterol moiety, the cholesterol-cholesterol interaction can operate cooperatively with the complementary base pairing. In addn., the gel fiber structure is clearly changed by the addn. of the adenine-appended cholesterol. Taking the fact that there is no report for such an additive effect inducing a structural change with maintaining the gel stability into consideration, the authors' attempt at combining cholesterol columnar stacks with the nucleobase additives provides a new methodol. to control the stability and the morphol. of organogels.
- IT 362-75-4, 2',3'-O-Isopropylidene adenosine
RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of uracil-appended cholesterol gelator and effects on gel stability and morphol. using complementary and non-complementary nucleobases)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34. ANSWER 2 OF 824 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:816750 HCAPLUS

DOCUMENT NUMBER: 138:39493

TITLE: Adenosine 5'-O-(1-Boranotriphosphate) Derivatives as Novel P2Y1 Receptor Agonists

AUTHOR(S): Nahum, Victoria; Zuendorf, Gregor; Levesque, Sebastien A.; Beaudoin, Adrien R.; Reiser, Georg; Fischer, Bilha
CORPORATE SOURCE: Department of Chemistry Gonda-Goldschmied Medical Research Center, Bar-Ilan University, Ramat-Gan, 52900, Israel

SOURCE: Journal of Medicinal Chemistry (2002), 45(24), 5384-5396

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:39493

AB P2-receptors (P2-Rs) represent important targets for novel drug development. Most ATP analogs proposed as potential drug candidates have short-comings such as limited receptor-selectivity and limited stability that justify the search for new P2-R agonists. Therefore, a novel series of nucleotides based on the adenosine 5'-O-(1-boranotriphosphate) (ATP-.alpha.-B) scaffold was developed and tested as P2Y1-R agonists. An efficient four-step one-pot synthesis of several ATP-.alpha.-B analogs from the corresponding nucleosides was developed, as well as a facile method for the sepn. of the diastereoisomers (A and B isomers) of the chiral products. The potency of the new analogs as P2Y1-R agonists was evaluated by the agonist-induced Ca²⁺ release of HEK 293 cells stably transfected with rat-brain P2Y1-R. ATP-.alpha.-B A isomer was equipotent with ATP (EC₅₀ = 2 .times. 10⁻⁷ M). However, 2-MeS- and 2-Cl- substitutions on ATP-.alpha.-B (A isomer) increased the potency of the agonist up to 100-fold, with EC₅₀ values of 4.5 .times. 10⁻⁹ and 3.6 .times. 10⁻⁹ M, compared to that of the ATP-.alpha.-B (A isomer).

Diastereoisomers A of all ATP-.alpha.-B analogs were more potent in inducing Ca²⁺ release than the corresponding B counterparts, with a 20-fold difference for 2-MeS-ATP-.alpha.-B analogs. The chem. stability of the new P2Y₁-R agonists was evaluated by ³¹P NMR under physiol. and gastric-juice pH values at 37 .degree.C, with rates of hydrolysis of 2-MeS-ATP-.alpha.-B of 1.38 .times. 10⁻⁷ s⁻¹ (t_{1/2} of 1395 h) and 3.24 .times. 10⁻⁵ s⁻¹ (t_{1/2} = 5.9 h), resp. The enzymic stability of the new analogs toward spleen NTPDase was evaluated. Most of the new analogs were poor substrates for the NTPDase, with ATP-.alpha.-B (A isomer) hydrolysis being 5% of the hydrolysis rate of ATP. Diastereoisomers A and B exhibited different stability, with A isomers being significantly more stable, up to 9-fold. Furthermore, A isomers that are potent P2Y₁-R agonists barely interact with NTPDase, thus exhibiting protein selectivity. Therefore, on the basis of our findings, the new, highly water-sol., P2Y₁-R agonists may be considered as potentially promising drug candidates.

IT 16658-10-9P 478702-40-8P 478702-41-9P

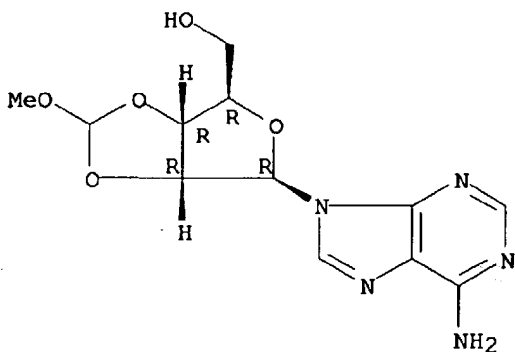
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of adenosine boranotriphosphate derivs. as novel P2Y₁ receptor agonists)

RN 16658-10-9 HCAPLUS

CN Adenosine, 2',3'-O-(methoxymethylene)- (9CI) (CA INDEX NAME)

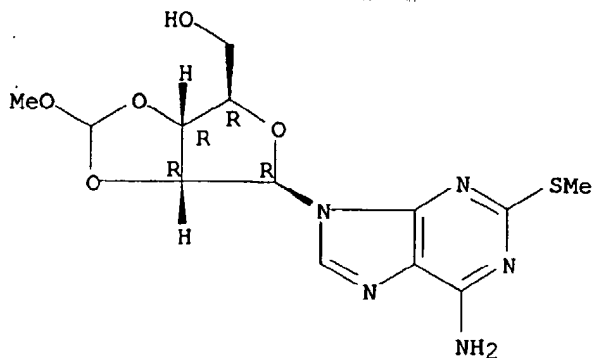
Absolute stereochemistry.



RN 478702-40-8 HCAPLUS

CN Adenosine, 2',3'-O-(methoxymethylene)-2-(methylthio)- (9CI) (CA INDEX NAME)

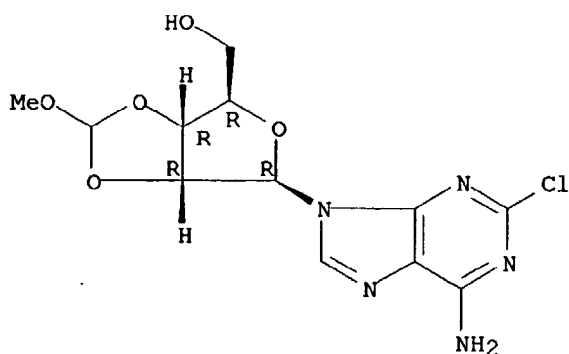
Absolute stereochemistry.



RN 478702-41-9 HCAPLUS

CN Adenosine, 2-chloro-2',3'-O-(methoxymethylene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 824 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:789678 HCAPLUS

DOCUMENT NUMBER: 138:24909

TITLE: Synthesis and Evaluation of Analogs of 5'-((Z)-4-Amino-2-butenyl)methylamino)-5'-deoxyadenosine as Inhibitors of Tumor Cell Growth, Trypanosomal Growth, and HIV-1 Infectivity

AUTHOR(S): Marasco, Canio J., Jr.; Kramer, Debora L.; Miller, John; Porter, Carl W.; Bacchi, Cyrus J.; Rattendi, Donna; Kucera, Louis; Iyer, Nathan; Bernacki, Ralph; Pera, Paula; Sufrin, Janice R.

CORPORATE SOURCE: Grace Cancer Drug Center, Department of Pharmacology and Therapeutics, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(23), 5112-5122

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English
 OTHER SOURCE(S): CASREACT.138:24909

AB A well-defined series of 5'-([(Z)-4-amino-2-butenyl]methylamino)-5'-deoxyadenosine analogs was designed and synthesized in order to further ascertain the optimal structural requirements for S-adenosylmethionine decarboxylase inhibition and potentially to augment and perhaps sep. their antiproliferative and antitrypanosomal activities. Most structural modifications had a deleterious affect on both the antitrypanosomal and antineoplastic activity of 5'-([(Z)-4-amino-2-butenyl]methylamino)-5'-deoxyadenosine. However, di-O-acetylation of the parent compd. produced a potential prodrug that caused markedly pronounced inhibition of trypanosomal and neoplastic cell growth and viability. Moreover, the acetylated deriv. of 5'-([(Z)-4-amino-2-butenyl]methylamino)-5'-deoxyadenosine did inhibit HIV-1 growth and infectivity, whereas the parent compd. did not.

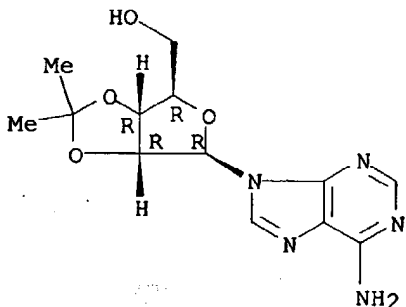
IT 362-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis and evaluation of analogs of aminobutenylmethylaminodeoxyadenosine as inhibitors of tumor cell growth trypanosomal growth and HIV infectivity)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 30685-38-2P

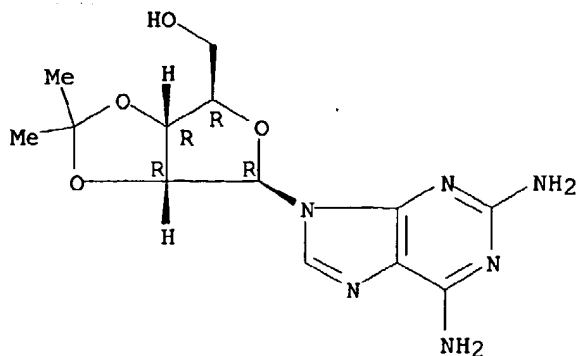
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and evaluation of analogs of aminobutenylmethylaminodeoxyadenosine as inhibitors of tumor cell growth trypanosomal growth and HIV infectivity)

RN 30685-38-2 HCAPLUS

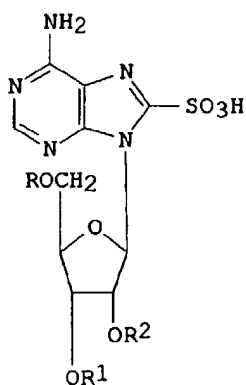
CN Adenosine, 2-amino-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 400 OF 824 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1985:95990 HCAPLUS
 DOCUMENT NUMBER: 102:95990
 TITLE: Synthesis of adenosine 8-sulfonic acid and some of its derivatives
 AUTHOR(S): Zavgorodnii, S. G.; Tsilevich, T. L.; Florent'ev, V. L.
 CORPORATE SOURCE: Inst. Mol. Biol., Moscow, USSR
 SOURCE: Bioorganicheskaya Khimiya (1984), 10(10), 1371-5
 CODEN: BIKHD7; ISSN: 0132-3423
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



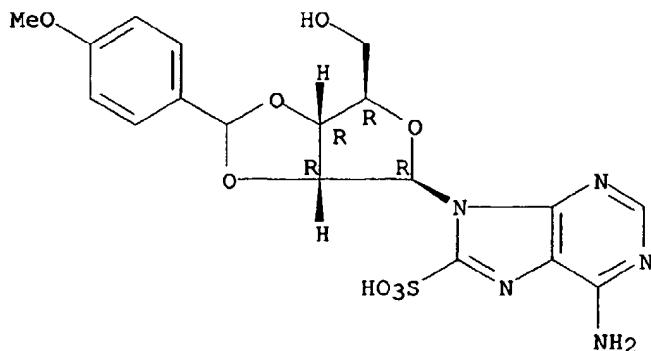
I

AB Adenosinesulfonic acids I [R = H, R1 = R2 = 4-MeOC6H4CH2; R-R2 = H; R = P(O)(OH)2, R1 = R2 = H; R = R2 = H, R1 = P(O)(OH)2; R = R1 = H, R2 = P(O)(OH)2; RR1 = P(O)(OH), R2 = H] were prepd. by treatment of the corresponding C-8 bromo derivs. with Na2SO3. I [R = (OH)2P(O)OP(O)(OH)OP(O)(OH), R1 = R2 = H; R = H, R1R2 = P(O)(OH)] were also prepd., and I possessed syn conformations in soln.

IT 94834-94-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 94834-94-3 HCAPLUS
CN 9H-Purine-8-sulfonic acid, 6-amino-9-[2,3-O-[(4-methoxyphenyl)methylene]-
.beta.-D-ribofuranosyl]-, monosodium salt (9CI) (CA INDEX NAME)

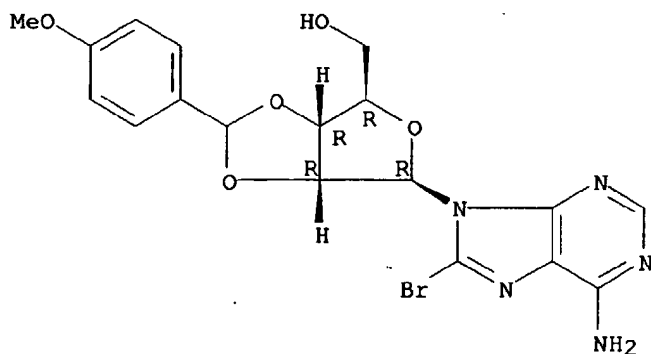
Absolute stereochemistry.



● Na

IT 92890-90-9
RL: RCT (Reactant); RACT. (Reactant or reagent)
(substitution reaction of, with sodium sulfite, sulfonic acid derivs.
from)
RN 92890-90-9 HCAPLUS
CN Adenosine, 8-bromo-2',3'-O-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



L34 ANSWER 401 OF 824 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:95979 HCAPLUS
DOCUMENT NUMBER: 102:95979
TITLE: Studies on chemical synthesis of antimetabolites. 33.

AUTHOR(S):
CORPORATE SOURCE:
SOURCE:

Studies directed toward the total synthesis of
sinefungin. I. Synthesis of 4-(5'-deoxyuridin-5'-yl)-
4-nitrobutyronitrile, 4-(5'-deoxyadenosin-5'-yl)-4-
nitrobutyramide and closely related nucleosides
Mizuno, Yoshihisa; Tsuchida, Kiyomi; Tampo, Hajime
Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan
Chemical & Pharmaceutical Bulletin (1984), 32(8),
2915-24

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The synthesis of 1-(5,6-dideoxy-6-nitro-.beta.-D-ribo-
hexofuranosyl)uracil, 9-(5,6-dideoxy-6-nitro-.beta.-D-ribo-
hexofuranosyl)adenine, 4-(5'-deoxyuridin-5'-yl)-4-nitrobutyronitrile and
4-(5'-deoxyadenosin-5'-yl)-4-nitrobutyramide from 2',3'-O-
isopropylideneuridine-5'-aldehyde (I) was achieved by aldol condensation
with MeNO₂ or O₂N(CH₂)₃CO₂Me, Michael reaction of I with CH₂:CHCN or
CH₂:CHCO₂Me, and conversion of the uracil nucleoside into the adenine
nucleoside by transglycosylation. The chem. developed for the prepn. of
these compds. should be useful in the total synthesis of the nucleoside
antibiotics sinefungin and A9145C, which are potent inhibitors of certain
S-adenosylmethionine-dependent methyltransferases.

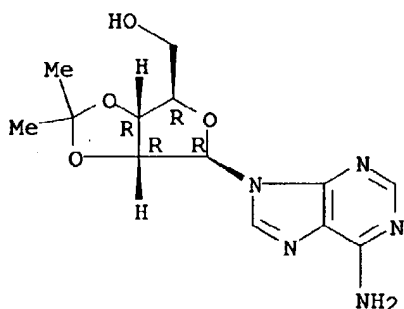
IT 362-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. and condensation of, with nitromethane)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 402 OF 824 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1985:46215 HCAPLUS

DOCUMENT NUMBER: 102:46215

TITLE: Cyclonucleoside formation and ring cleavage in the
reaction of 2',3'-O-isopropylideneadenosine with
benzoyl chloride and its substituted derivatives

AUTHOR(S): Anzai, Kentaro; Uzawa, Jun

CORPORATE SOURCE: Inst. Phys. Chem. Res., Wako, 351, Japan

SOURCE: Journal of Organic Chemistry (1984), 49(26), 5076-80

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal

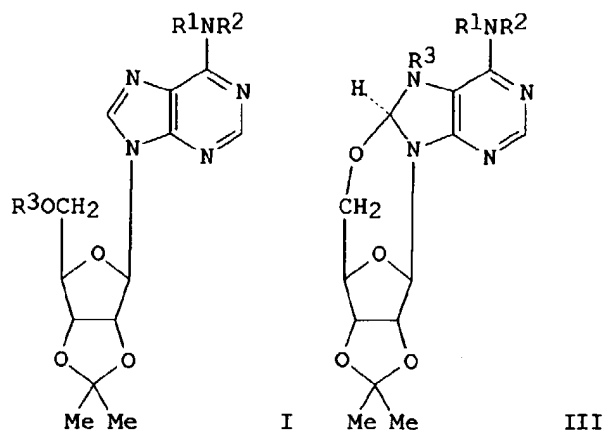
LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 102:46215

GI



AB Reaction conditions suitable for the formation of 8,5'-O-cycloadenosine derivs. in the reaction of isopropylideneadenosine I ($R_1 = R_2 = R_3 = H$) (II) BzCl and substituted benzoyl chlorides were investigated. Thus, reaction of II with p-toluoyl chloride in a CH_2Cl_2 -Et₃N mixt. afforded 8,5'-O-cyclonucleosides III ($R_1 = R_2 = R_3 = p\text{-MeC}_6\text{H}_4\text{CO}$) (34%) and III ($R_1 = H$, $R_2 = R_3 = p\text{-MeC}_6\text{H}_4\text{CO}$) (11%), a noncyclized acylate I ($R_1 = R_2 = R_3 = p\text{-MeC}_6\text{H}_4\text{CO}$) (30%), and a ring-cleaved imidazole compd. (12%). The structures of these compds. were detd. by ¹³C NMR.

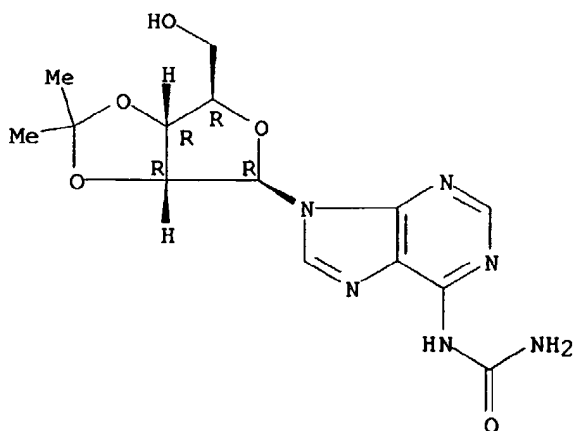
IT 93135-59-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 93135-59-2 HCAPLUS

CN Adenosine, N-(aminocarbonyl)-2',3'-O-(1-methylethylidene)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



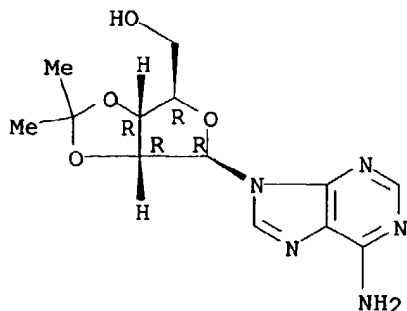
IT 362-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzoyl chlorides, cyclization in)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 821 OF 824 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1961:93506 HCAPLUS

DOCUMENT NUMBER: 55:93506

ORIGINAL REFERENCE NO.: 55:17640c-f

TITLE: Synthesis of nucleotide coenzymes and related compounds

AUTHOR(S): Shabarova, Z. A.; Ryabova, T. S.; Prokof'ev, M. A.

CORPORATE SOURCE: M. V. Lomonosov State Univ., Moscow

SOURCE: Doklady Akad. Nauk S.S.S.R. (1961), 136, 1116-19

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

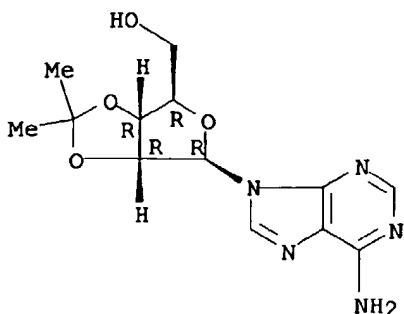
AB cf. CA 54, 11040h; Moffatt and Kharana, CA 53, 5274b. Me ester of N-(2',3'-isopropylideneadenosine-5'-benzylphosphorophenylalanine hydrogenated in EtOH in the presence of Et₃N over Pd black gave 70% corresponding phosphate, isolated as the Et₃N salt (I), m. 92-4.degree. (decompn.), R_f 0.47 in satd. aq. BuOH. Stirring Ba ribose 5-phosphate with ion exchange resin KU-2 (H-form) in H₂O gave after neutralization with Bu₃N, tributylammonium ribose 5-phosphate (II); similarly were prepd. tributylammonium glucose 6-phosphate (IIA) and tributylamine salts of H₃PO₄ and H₄P₂O₇. I treated with HCl in dioxane, the mixt. filtered, treated with a pyridine soln. of II, kept 3 days at room temp., and chromatographed in 96% EtOH-0.5M NH₄OAc gave spots, of which one was caused by 2',3'-isopropylideneadenosine 5'-diphosphoribose (III), while the 2nd spot was of lower R_f. This was eluted and refluxed briefly with 0.01N HCl and again chromatographed, showing spots indicative of adenosine, ribose, adenosine diphosphate, and adenosine 5'-phosphate. Yield of III was estd. at 25%. I similarly treated with IIA 3 days gave 37% (estd.) 2',3'-isopropylideneadenosine 5'-diphosphoglucose (R_f 0.47 in 96% EtOH-0.5M NH₄OAc), along with the adenosine 5'-monophosphate. Similarly, I and Bu₃N phosphate or pyrophosphate gave 27-39% isopropylideneadenosine di- and triphosphates, detected electrophoretically.

IT 362-75-4, Adenosine, 2',3'-O-isopropylidene-
(phosphates)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 822 OF 824 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1961:93503 HCAPLUS

DOCUMENT NUMBER: 55:93503

ORIGINAL REFERENCE NO.: 55:17637i,17638a-i,17639a-d

TITLE: High-energy phosphates. X. The preparation of triesters of pyrophosphoric acid and their use in the synthesis of nucleotide derivatives

AUTHOR(S): Cramer, Friedrich; Wittmann, Rolf

CORPORATE SOURCE: Univ. Heidelberg, Germany

SOURCE: Chem. Ber. (1961), 94, 328-37

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Triesters of pyrophosphoric acid, obtainable from (EtO)2P(O)OC(OEt):CHCO2Et (I) and monoesters of H3PO4, react with amines, alcs., and acid anions with the transfer of the monoester moiety. P1-(15-Adenosyl) P2-diethyl pyrophosphate (II) behaved as an activated adenosinephosphoric acid and transferred the nucleotide residue to bases, alcs., and acids. PhOP(O)(OH)2 (III) (0.348 g.) and 1.48 g. I in 10 cc. Et2O kept 1 hr. at 20.degree., treated with 5 cc. CHCl3 and 3 cc. cyclohexylamine, filtered after 24 hrs. from 0.087 g. bis(cyclohexylammonium) salt of [(PhO)P(O)(OH)]2O, concd. to 5 cc., and treated with petr. ether gave 0.518 g. cyclohexylamine salt (IV) of the cyclohexylamide of III, m. 192-3.degree. (CHCl3-petr. ether). III treated in the usual manner with I, the resulting triester treated after 1 hr. with cooling with dry NH3, and filtered, the residue washed with dry Et2O and dissolved in MeOH, and the soln. treated with a small amt. of cyclohexylamine, filtered, concd., treated with C, and dild. with Et2O yielded 0.296 g. cyclohexylamine salt (V) of the amine of III, m. 220-7.degree. (with sintering at 179-84.degree.) resolidifying and remelting at 237-40.degree.. Similar results were obtained with PhNH2 and p-O2NC6H4NH2. II (0.348 g.) and 1.48 g. I in 10 cc. Et2O kept 1 hr. at 20.degree., treated with 3 cc. PhCH2OH and 5 cc. C5H5N, dild. after 48 hrs. with dil. NH4OH and extd. with Et2O, the ext. reextd. with NH4OH, the aq. phase treated with 2 cc. cyclohexylamine, concd. at 45.degree. with occasional removal of the ppt. by filtration, the resulting sirup dissolved in 50 cc. CHCl3, the soln. washed with H2O, combined with the original filter residue, dissolved in Me2CO, and dild. with petr. ether yielded 0.562 g. cyclohexylamine salt of PhCH2O(PhO)P(O)OH, m. 147-9.degree. (repptd. from CHCl3-Me2CO with petr. ether). The triester

from III and I treated 48 hrs. at 50.degree. with 0.74 g. BuOH in 4 cc. C5H5N, concd., treated with 2 cc. cyclohexylamine and 30 cc. H2O, and worked up yielded 0.509 g. cyclohexylamine salt of PhO(BuO)P(O)OH (VI), m. 110-11.degree. (Me2CO-CHCl3-petr. ether). Similar results were obtained with iso-PrOH and p-O2NC6H4CH2OH. III (0.348 g.) in 10 cc. dry Et2O treated with 1.480 g. I and after 1 hr. at 20.degree. with 0.10 g. isopropylidenadenosine (from adenosine and Me2CO with ZnCl2), kept 48 hrs. at 20.degree. and 6 hrs. at 40.degree., concd. in vacuo at 45.degree., dissolved in a little dil. NH4OH, washed with Et2O, treated with 1 cc. cyclohexylamine, concd. in vacuo at 40.degree., dissolved in Me2CO, filtered, treated with 20 cc. H2O, washed with CHCl3, and evapd. in vacuo, and the residue repptd. several times from Me2CO with petr. ether yielded 0.096 g. Ph isopropylideneadenosine-5'-phosphate (VII), m. 210-12.degree.. Anhyd. H3PO4 (0.196 g.), 0.404 g. Et3N, 5 cc. PhCH2OH, and 1.48 g. I kept 48 hrs. at 40.degree., dild. with 20 cc. Et2O and extd. with dil. NH4OH, and ext. passed through a column of Amberlite IR-120 in NH4OH, the eluate evapd., the residue extd. with 98% EtOH, the ext. concd. and dild. with Me2CO, the ppt. dissolved in 3N H2SO4 and extd. with Et2O, and the ext. treated with excess cyclohexylamine gave 0.352 g. salt of PhCH2OP(O)(OH)2, m. 232-5.degree.. Anhyd. H3PO4 (0.196 g.) in 10 cc. PhCH2OH and 2.96 g. I kept 72 hrs. at 40.degree., dild. with 20 cc. Et2O and extd. with dil. NH4OH, and the ext. treated with cooling with 3N H2SO4 yielded 0.268 g. (PhO)2P(O)OH, m. 78.degree.. III (0.348 g.) in 2 cc. C5H5N and 0.74 g. I kept 48 hrs. at 40.degree., dild. with 50 cc. H2O, and treated with 2 cc. cyclohexylamine gave 0.38 g. bis(cyclohexylamine) salt (VIII) of [(PhO)(HO)P(O)]2O, m. 255-8.degree. (cor.) (H2O). Similarly were prepd. the bis(cyclohexylamine) salt (IX) of [(p-ClC6H4O)(HO)P(O)]2O, m. 276-9.degree. (cor.), and the bis(cyclohexylamine) salt (X) of [(p-MeC6H4O)(HO)P(O)]2O, m. 270-3.degree. (cor.), in 73.8 and 78.4% yield, resp. The triester from III and I treated after 1 hr. with 50 cc. Et2O and with cooling with 0.428 g. 2,6-lutidine, the Et2O phase decanted after 10 min., the residue washed with cold Et2O, treated with 0.832 g. p-ClC6H4OP(O)(OH)2 in 5 cc. C5H5N, kept 6 hrs. at 40.degree., and evapd. in vacuo, and the residue dissolved in H2O, passed through Amberlite IR-120, and added to aq. cyclohexylamine gave 0.415 g. bis(cyclohexylamine) salt (XI) of p-ClC6H4O(HO)P(O)OP(O)(OH)OPh, m. 262.degree. (cor.) (aq. EtOH-C5H5N). (EtO)2P(O)(OPh)OH and H3PO4 gave similarly PhO(HO)P(O)OP(O)(OH)2 (XII). III (0.348 g.) in 10 cc. Et2O and 1.48 g. I kept 1 hr. at 20.degree., treated with 2.44 g. BzOH in 15 cc. C5H5N, kept 14 hrs. at 40.degree., and evapd. in vacuo, the residue dissolved in 20 cc. H2O, washed with 20 cc. Et2O, stirred 3 hrs. with 2 cc. PhNH2, and extd. with Et2O gave 0.137 g. (PhO)(BzO)P(O)OH, m. 161.degree.. Adenosine-5'-phosphoric acid (0.694 g.), 0.74 g. Bu3N, and 0.296 g. I in 20 cc. dry HCONMe2 stirred 2-3 hrs. at 20.degree., dild. with about 150 cc. dry Me2CO, treated with 0.6 g. NaI in Me2CO, and centrifuged gave 0.912 g. Na salt (XIII) of II.H2O. XIII (0.261 g.) in 2 cc. abs. MeOH and 1 cc. dry C5H5N kept 3 hrs. at 50.degree., concd., chromatographed (descending) 16 hrs. with 7:1:2 iso-PrOH-NH3-H2O (solvent A) on Whatman 3MM paper, the band, Rf 0.35, cut out and eluted with 300 cc. MeOH in small portions, and the eluate concd., filtered, dild. with Me2CO and Et2O, and centrifuged yielded 0.157 g. NH4 salt of Me adenosine 5'-phosphate-H2O (XIV). XIII (0.261 g.) in 2 cc. dry HCONMe2 and 0.396 g. cyclohexylamine kept 12 hrs. at 20.degree. and evapd. in vacuo at 35.degree., and the residue chromatographed on paper gave 0.206 g. NH4 salt of adenosine-5'-phosphoric acid cyclohexylamide-4H2O (XV), Rf 0.52. XIII (0.261 g.), 0.87 g. III, 2 cc. HCONMe2, and 2 cc. C5H5N kept 48 hrs. at 20.degree. and evapd. in vacuo at 35.degree., the residue dissolved in

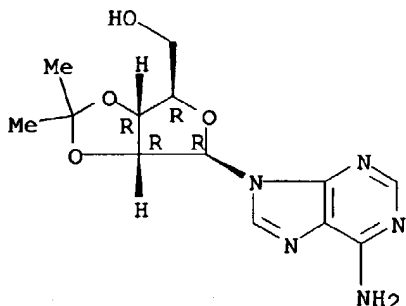
a little H₂O, treated with 2 cc. cyclohexylamine, dild. with 200 cc. MeOH and some Me₂CO, filtered, and evapd., and the residue chromatographed in the usual manner on paper gave 0.242 g. di-NH₄ P1-(5'-adenosyl) P2-phenyl pyrophosphate-5H₂O (XVI), R_f 0.36. XIII (0.262 g.) in 2 cc. dry C₅H₅N, 0.61 g. BzOH, 0.505 g. Et₃N, and 1 cc. C₅H₅N kept 12 hrs. at 40.degree., treated 2 hrs. with 2 cc. PhNH₂, and worked up gave 0.034 g. adenosine-5'-phosphoric benzoic anhydride, m. 159-61.degree.. The R_f values with 8:1:1 iso-PrOH-concd. NH₄OH-H₂O were detd. (descending) for the following compds.: III 0.08, p-ClC₆H₄OP(O)(OH)₂ 0.14, p-MeC₆H₄OP(O)(OH)₂ 0.09, (EtO)₂P(O)OH 0.58, PhCH₂O(PhO)P(O)OH 0.73, VI 0.73, p-O₂NC₆H₄O(PhO)P(O)OH 0.69, IV 0.72, benzylamide of III 0.65, anilide of III 0.64, p-nitrilanilide of III 0.67, V 0.38, VIII 0.42, IX 0.51, X 0.45, XI 0.45, XII 0.02, I, 0.60 and 0.89, isopropylideneadenosine 0.69, VII 0.55. The R_f values with solvent A and with 2:1 iso-PrOH-1% aq. (NH₄)₂SO₄ (given in this order) were detd. for the following compds.: adenosine-5'-phosphoric acid (XVII), 0.10, 0.34; 3'-isomer of XVII, 0.14, 0.43; diadenosyl pyrophosphate, 0.11, 0.25; XIII, 0.22-0.56, 0.62; amide of XVII, 0.22, 0.32; XV, 0.54, 0.68; XIV, 0.35, 0.45; XVI, 0.37, 0.46.

IT 362-75-4, Adenosine, 2',3'-O-isopropylidene-
(prepn. of)

RN 362-75-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 823 OF 824 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1959:2115 HCAPLUS

DOCUMENT NUMBER: 53:2115

ORIGINAL REFERENCE NO.: 53:401g-i,402a-g

TITLE: Synthesis of 6-(dimethylamino)-9-(.beta.-D-ribofuranosyl)purine 5'-phosphate

AUTHOR(S): Andrews, K. J. M.; Barber, W. E.

CORPORATE SOURCE: Roche Products Ltd., Welwyn Garden City, UK

SOURCE: J. Chem. Soc. (1958) 2768-71

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB To 16 g. 6-(dimethylamino)-2-(methylthio)purine in 100 ml. EtOH was added 38 ml. aq. 2N NaOH followed by 22 g. HgCl₂ in 100 ml. EtOH, and the solid filtered off, washed with H₂O, EtOH, and Et₂O, and dried giving 25 g. HgCl complex (I). I (13.5 g.) and 13.5 g. Hyflo Supercel (IA) in 250 ml. PhCl was distd. to remove half the PhCl (and residual H₂O), treated with acetochlororibofuranose (II) [from 12 g. tetra-O-acetyl-.beta.-D-ribofuranose (IIA)] in 100 ml. dry PhCl, stirred and refluxed 3 hrs.,

filtered hot, the insol. material extd. with hot CHCl_3 until the exts. were colorless, the combined PhCl-CHCl_3 solns. evapd. in vacuo and the residue dissolved in 150 ml. CHCl_3 , the CHCl_3 soln. washed with 2 50-ml. portions 30% aq. KI, then H_2O , dried, treated with C, and evapd. in vacuo giving 16.3 g. yellow-brown glass (III). The III in 25 ml. dry MeOH and 200 ml. 5N MeOH- NH_3 kept 24 hrs. at room temp. then evapd. in vacuo gave 4.2 g. 6-(dimethylamino)-2-(methylthio)-9-(β -D-ribofuranosyl)purine, m. 174-5.degree. (H_2O), [α]20D -43.6.degree. (c 1.6, MeOH). The III (crude 6-dimethylamino-2-(methylthio)-9-[(2',3',5'-tri-O-acetyl)- β -D-ribofuranosyl]purine from 32 g. I and 28 g. II) in 1.5 l. MeOH and about 80 g. freshly prepd. Raney Ni stirred and refluxed 1 hr., filtered through IA, the filtrate evapd. in vacuo, the residual gum, 300 ml. MeOH, and 3 ml. N MeONa refluxed 1 hr. (pH kept above 8 by adding more MeONa, if necessary), evapd. to dryness, the residue dissolved in a few ml. H_2O , the H_2O soln. dild. with boiling Me_2CO , the Me_2CO soln. dild. with boiling Me_2CO , the Me_2CO soln. evapd. in vacuo, the Me_2CO evapns. repeated twice, and the solid product recrystd. from H_2O and Me_2CO gave 12.1 g. 6-dimethylamino-9-(β -D-ribofuranosyl)purine (IV), fluffy needles, m. 182-3.degree., [α]20D -58.5.degree. (c 2.3, H_2O). IV (9 g.), 450 ml. dry Me_2CO , 36 g. anhyd. CuSO_4 , and 36 g. p-MeC $_6$ H $_4$ SO $_3$ H in 200 ml. Me_2CO stirred 0.5 hr., filtered, the insol. washed with Me_2CO , the combined filtrate and washings poured into 30 g. anhyd. Na_2CO_3 in 400 ml. H_2O , extd. with CHCl_3 , and the CHCl_3 exts. evapd. in vacuo gave 6.8 g. 6-dimethylamino-9-[(2',3'-O-isopropylidene)- β -D-ribofuranosyl]purine (V), needles, m. 176-7.degree. (EtOH). To 4.07 g. $\text{PhCH}_2\text{P}(\text{OH})_2$ in 33 ml. dry C $_6$ H $_6$ was added 4.9 g. Ph_2PCl , stirred, 3.33 g. Et $_3\text{N}$ in 33 ml. dry C $_6$ H $_6$ added in 10 min., stirred 1 hr. at room temp., the Et $_3\text{N.HCl}$ filtered off, the filtrate treated with 5 g. dry V and 2.7 ml. 2,6-lutidine, stirred 0.5 hr. at room temp., filtered, the filtrate evapd. in vacuo at room temp., the residue dissolved in 100 ml. CHCl_3 , the CHCl_3 soln. washed with H_2O , satd. aq. NaHCO_3 , and H_2O , dried, and evapd. in vacuo at room temp. giving 7.8 g. crude 6-dimethylamino-9-[(2',3'-O-isopropylidene)- β -D-ribofuranosyl]purine 5'-benzyl H phosphite (VI), pale yellow oil. The VI in 80 ml. dry C $_6$ H $_6$ and 2 g. N-chlorosuccinimide was stirred 2 hrs. at room temp., 80 ml. MeCN and 160 ml. satd. aq. NaHCO_3 soln. added, stirred 6 hrs., kept 9 hrs., the aq. phase sepd., filtered, and the filtrate freed of residual MeCN by evapn. in vacuo below 30.degree.; half of the residual aq. soln. was cooled in ice H_2O , the pH adjusted to about 2 and extd. with CHCl_3 , the CHCl_3 exts. dried, evapd. in vacuo at room temp., the residue (2.2 g.) immediately dissolved in 100 ml. EtOH, 100 ml. H_2O added, the soln. treated with C, filtered, the filtrate hydrogenated (2 hrs.) over 0.5 g. PdO $_2$ and 0.5 g. 10% Pd-C, filtered, the filtrate evapd. in vacuo, the residue refluxed 2 min. with 3 ml. H_2O to remove the isopropylidene group, cooled, dild. to turbidity with Me_2CO , and set aside 3 days at 0.degree. gave 0.5 g. 6-dimethylamino-9-(β -D-ribofuranosyl)purine 5'-phosphate (VIII), m. 225.degree. (decompn.), [α]20D -51.degree. (c 1.98, H_2O), λ 268 m. μ . (ϵ 18,300), Rf 0.39, ultraviolet absorbent, contains P, developed with PROH-aq. NH_3 (d. 0.88)- H_2O (60:30:10). To 10 g. 4,5-diamino-6-(dimethylamino)-2-(methylthio)pyrimidine in 400 ml. 2N AcONa, 25 ml. 2N HCl, and 5 ml. AcOH at 80.degree. was added 20 g. NaNO_2 in 200 ml. H_2O , kept 0.5 hr. at 95.degree., and cooled giving 9.3 g. 6-(dimethylamino)-2-(methylthio)-8-azapurine (VIII), needles, m. 262.degree.; the VIII HgCl_2 complex, prepd. as above (12 g.), and II (from 9.5 g. IIA as above) gave the crude tri-O-acetylribosyl compd. which deacetylated with MeOH- NH_3 gave 49.5% 6-(dimethylamino)-2-(methylthio)-9-(β -D-ribofuranosyl)-8-azapurine (IX), m. 146.5-8.degree. (H_2O). IX (400 mg.), 100 ml. EtOH, and about 3

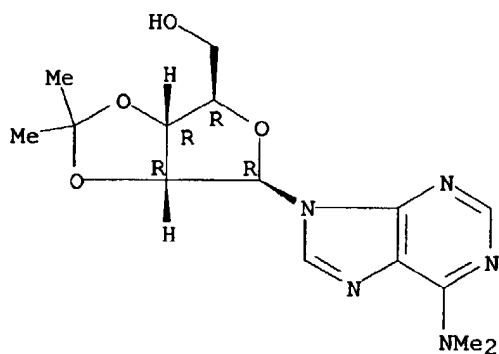
g. Raney Ni refluxed 1 hr., filtered through IA, and the filtrate evapd. in vacuo gave 70 mg. 6-(dimethylamino)-9-(.beta.-D-ribofuranosyl)-8-azapurine, m. 216.degree. (aq. EtOH). IV (290 mg.), 37 ml. dry BzH, and 750 mg. ZnCl₂ shaken 24 hrs., poured into 50 ml. dry Et₂O, the solid filtered off, dissolved in 4.3 ml. EtOCH₂CH₂OH, the soln. treated with 3.2 ml. 2N aq. NaOH, kept 10 min., filtered, and the filtrate evapd. in vacuo gave 100 mg. 6-(dimethylamino)-9-[(2',3'-O-benzylidene)-.beta.-D-ribofuranosyl]purine, m. 172.degree. (EtOH). IV showed possibly a slight but not appreciable activity against Sarcoma 180; on a molar basis this activity was of the same order as for the purine. The activity of VII is under investigation.

IT 19083-21-7, Adenosine, 2',3'-O-isopropylidene-N,N-dimethyl-
(and derivs.)

RN 19083-21-7 HCAPLUS

CN Adenosine, N,N-dimethyl-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

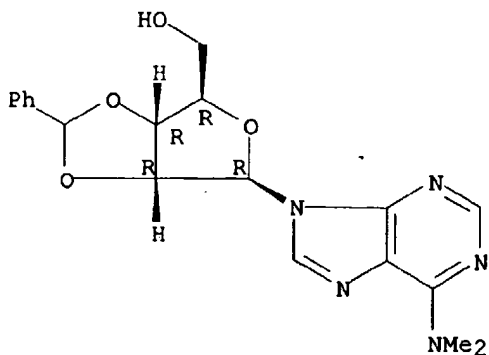


IT 110422-67-8, Adenosine, 2',3'-O-benzylidene-N,N-dimethyl-
(prepn. of)

RN 110422-67-8 HCAPLUS

CN Adenosine, 2',3'-O-benzylidene-N,N-dimethyl- (6CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 824 OF 824 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1958:113751 HCAPLUS
DOCUMENT NUMBER: 52:113751
ORIGINAL REFERENCE NO.: 52:20177g-i,20178a-b
TITLE: Purine N-oxides. I. Monooxides of aminopurines
AUTHOR(S): Stevens, Marcus A.; Magrath, David I.; Smith, Herman
W.; Brown, George Bosworth
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY
SOURCE: J. Am. Chem. Soc. (1958), 80, 2755-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

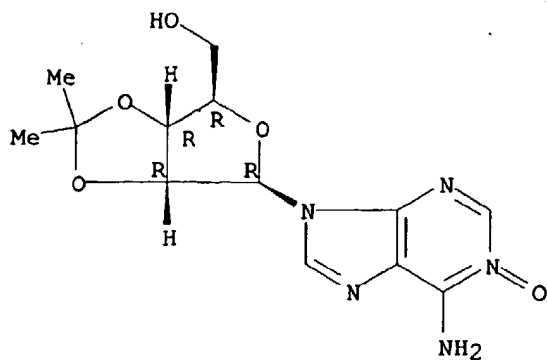
AB N-Monooxides were isolated from the mixts. resulting from the oxidation of adenine, adenosine, 2',3'-isopropylideneadenosine (I), or 2,6-diaminopurine with H₂O₂-AcOH. Adenine (10 g.) in 60 ml. hot AcOH cooled to 20.degree., 37 ml. 30% H₂O₂ added, the soln. held at room temp. 4.5 days, and filtered yielded 84% adenine N-oxide (II), decomp. 297-307.degree.. II (250 mg.) in 100 ml. H₂O contg. 1 ml. NH₄OH shaken 6 hrs. with 3 ml. Raney Ni under 1 atm. H yielded 220 mg. adenine, m. 350.degree.. Anhyd. adenosine (10 g.) in 500 ml. AcOH and 50 ml. 30% H₂O₂ held 6 days at room temp., cooled in an ice bath, stirred with 4 g. 5% Pd-C, filtered, and the filtrate evapd. to 250 ml. in vacuo, and allowed to evap. yielded 10.8 g. adenosine N-oxide (III), m. 155.degree., decomp. 160.degree.. III (30 mg.) in N HCl refluxed 15 min. yielded II. I (2.0 g.) in 100 ml. AcOH and 10 ml. 30% H₂O₂ held 5 days at room temp., stirred 1 day with 0.5 g. 10% Pd-C at 20.degree., filtered, evapd. in vacuo at room temp., the residue in 15 ml. hot EtOH treated with C, cooled, the resulting gel warmed with 10 ml. EtOH, and the soln. cooled slowly yielded 845 mg. 2',3'-isopropylidene N-oxide (IV), m. 176-8.degree. (decompn.). IV (5 mg.) in 2 ml. N HCl boiled 2 min. yielded about 60% II. 2,6-Diaminopurine (V) (410 mg.) in 23 ml. AcOH and 1.8 ml. 30% H₂O₂ stirred 3 days at 25-30.degree., the soln. cooled to 0.degree., stirred 1 day at room temp. with 125 mg. 10% Pd-C, filtered, the filtrate evapd. to dryness in vacuo at 25-30.degree., the residue in 10 ml. H₂O dissolved by addn. of NH₄OH, the soln. dild. to 2 l., the pH adjusted to 10.8, chromatographed on Dowex-1, and eluted with NH₄Cl yielded 13.5% 2,6-diaminopurine N-oxide (VI). VI (7.5 mg.) hydrogenated over Raney Ni gave V.

IT 5167-12-4, Adenosine, 2',3'-O-isopropylidene-, 1-oxide
(prepn. of)

RN 5167-12-4 HCAPLUS

CN Adenosine, 2',3'-O-(1-methylethylidene)-, 1-oxide (9CI) (CA INDEX NAME)

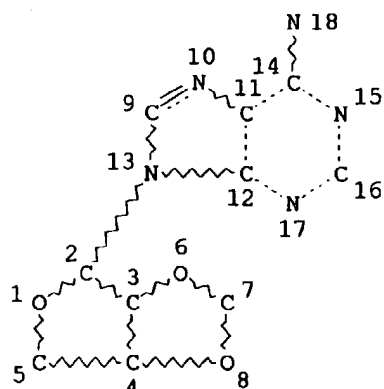
Absolute stereochemistry.



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STR



NODE ATTRIBUTES:

NSPEC IS RC AT 18
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

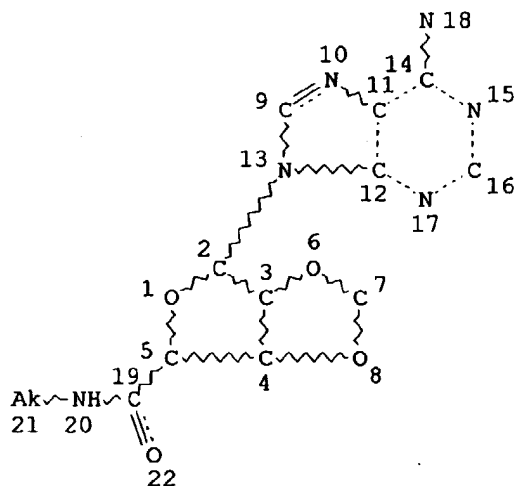
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L2 3214 SEA FILE=REGISTRY SSS FUL L1

L18 STR



NODE ATTRIBUTES:

NSPEC IS RC AT 18
 CONNECT IS E3 RC AT 5
 CONNECT IS E1 RC AT 21
 DEFAULT MLEVEL IS ATOM
 GGCAT IS LOC AT 21

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L19 246 SEA FILE=REGISTRY SUB=L2 SSS FUL L18
L35 63 SEA FILE=HCAPLUS ABB=ON PLU=ON L19

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Refs. Printed*

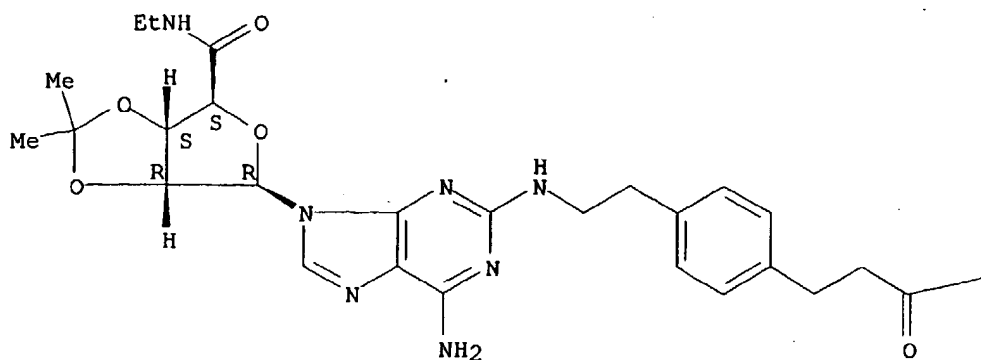
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L35 ANSWER 1 OF 63 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:271942 HCAPLUS
DOCUMENT NUMBER: 136:291358
TITLE: Diagnostic uses of 2-substituted adenosine
carboxamides
INVENTOR(S): Leung, Edward
PATENT ASSIGNEE(S): King Pharmaceuticals Research and Development, Inc.,
USA
SOURCE: U.S., 17 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6368573	B1	20020409	US 1999-440330	19991115
PRIORITY APPLN. INFO.:			US 1999-440330	19991115
OTHER SOURCE(S): MARPAT 136:291358				
AB The invention concerns a method for measuring myocardial function in a mammal in need of such measurement by: (a) administering 2-substituted adenosine carboxamide derivs. at a dosage rate of less than 1 .mu.g/kg/min, preferably between about 0.01 and 1 .mu.g/kg/min; and then: (b) performing a technique on the mammal to detect myocardial function. The method can be used to diagnose myocardial dysfunction by electrophysiol. anal. or by imaging the vasculature of the heart, esp. under conditions that simulate stress.				
IT 120225-76-5				
RL: ADV (Adverse effect, including toxicity); DGN (Diagnostic use); BIOL (Biological study); USES (Uses) (diagnostic uses of 2-substituted adenosine carboxamides)				
RN 120225-76-5 HCAPLUS				
CN Benzenepropanoic acid, 4-[2-[[6-amino-9-[N-ethyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranuronamidosyl]-9H-purin-2-yl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)				

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

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REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 2 OF 63 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:904207 HCAPLUS

DOCUMENT NUMBER: 136:37902

TITLE: Preparation of 2-aminocarbonyl-9H-purine nucleosides and their uses in treatment of respiratory disease, as A2a receptor agonists and anti-inflammatory agents

INVENTOR(S): Mantell, Simon John; Stephenson, Peter Thomas

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: PCT Int. Appl., 198 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001094368	A1	20011213	WO 2001-IB973	20010605
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,				

RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
 UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 US 2002058641 A1 20020516 US 2001-874007 20010605
 EP 1292604 A1 20030319 EP 2001-934242 20010605
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 PRIORITY APPLN. INFO.: GB 2000-14048 A 20000606
 GB 2000-18246 A 20000725
 GB 2000-24920 A 20001011
 US 2000-214307P P 20000627
 US 2000-225236P P 20000815
 US 2000-245243P P 20001102
 WO 2001-IB973 W 20010605
 OTHER SOURCE(S): MARPAT 136:37902
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 2-Aminocarbonyl-9H-purine nucleosides I wherein R, R2 are independently H, alkyl; R1 is H, substituted alkyl, fluorenyl; R3 is H, alkyl, cycloalkyl, benzyl; R4 is substituted azetidin-3-yl, pyrrolidin-3-yl, piperidin-3-yl, piperidin-4-yl, homopiperidin-3-yl or homopiperidin-4-yl; R3R4 taken together with the nitrogen atom to which they are attached, represent azetidiny, pyrrolidinyl, piperidinyl, piperazinyl, homopiperidinyl or homopiperazinyl, each being optionally substituted on a ring nitrogen or carbon atom by alkyl or cycloalkyl; R5 is CH2OH, amide; X is substituted alkylene; RX or R2X with the nitrogen atom to which they are attached, represent azetidin-3-yl, pyrrolidin-3-yl, piperidin-3-yl, piperidin-4-yl, homopiperidin-3-yl or homopiperidin-4-yl; Y is CO, CS, SO2, C=N(CN); were prepd. as A2a receptor agonists and anti-inflammatory agents. Thus, nucleoside II was prepd. and tested as A2a receptor agonist and anti-inflammatory agent. Title compds. were tested for biol. activity as A2a receptor agonists and anti-inflammatory agents and all were found to have an IC50 of less than 100 nM.

IT 380222-92-4P 380222-93-5P 380222-94-6P

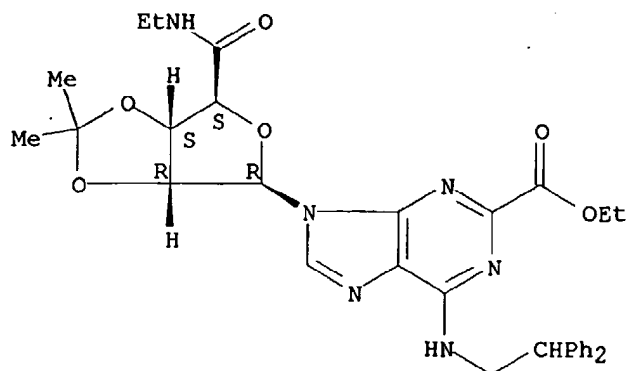
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 2-aminocarbonyl-9H-purine nucleosides and uses in treatment of respiratory disease, as A2a receptor agonists and anti-inflammatory agents)

RN 380222-92-4 HCAPLUS

CN 9H-Purine-2-carboxylic acid, 6-[(2,2-diphenylethyl)amino]-9-[N-ethyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranuronamidosyl]-, ethyl ester (9CI) (CA INDEX NAME)

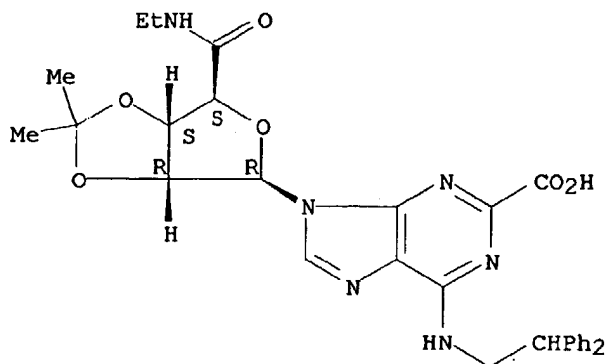
Absolute stereochemistry.



RN 380222-93-5 HCAPLUS

CN 9H-Purine-2-carboxylic acid, 6-[(2,2-diphenylethyl)amino]-9-[N-ethyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranuronamidosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

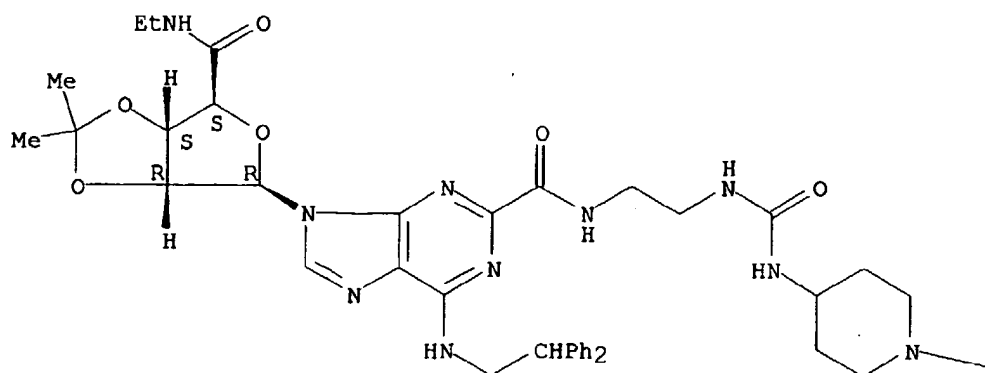


RN 380222-94-6 HCAPLUS

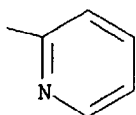
CN .beta.-D-Ribofuranuronamide, 1-deoxy-1-[6-[(2,2-diphenylethyl)amino]-2-[[[2-[[[1-(2-pyridinyl)-4-piperidinyl]amino]carbonyl]amino]ethyl]amino]carbonyl]-9H-purin-9-yl]-N-ethyl-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 3 OF 63 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:872195 HCAPLUS

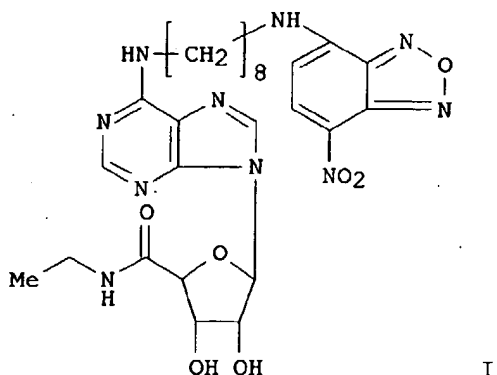
DOCUMENT NUMBER: 136:163634

TITLE: 7-Nitrobenzofurazan (NBD) derivatives of 5'-N-ethylcarboxamidoadenosine (NECA) as new

AUTHOR(S): fluorescent probes for human A3 adenosine receptors
Macchia, Marco; Salvetti, Francesca; Bertini, Simone;
Di Bussolo, Valeria; Gattuso, Lisa; Gesi, Marco;
Hamdan, Mahmoud; Klotz, Karl-Norbert; Laragione,
Teresina; Lucacchini, Antonio; Minutolo, Filippo;
Nencetti, Susanna; Papi, Chiara; Tuscano, Daniela;
Martini, Claudia

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita di
Pisa, Pisa, 56126, Italy

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AB New fluorescent ligands for adenosine receptors (ARs), obtained by the insertion, in the N6 position of NECA, of NBD-moieties with linear alkyl spacers of increasing length, proved to possess a high affinity and selectivity for the A3 subtype expressed in CHO cells. In fluorescence microscopy assays, compd. I, the most active and selective for human A3-AR, permitted visualization and localization of this human receptor subtype, showing its potential suitability for internalization and trafficking studies in living cells.

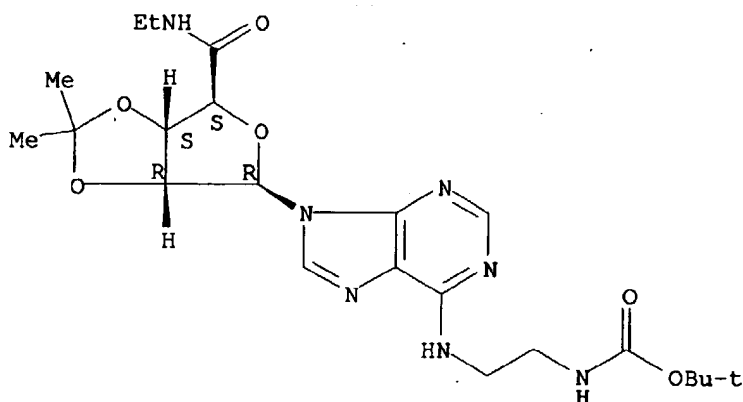
IT 396718-59-5P 396718-60-8P 396718-61-9P
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396718-71-1P 396718-75-5P 396718-77-7P
396718-79-9P 396718-81-3P 396718-83-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(nitrobenzofurazan derivs. of ethylcarboxamidoadenosine as fluorescent probes for human A3 adenosine receptors)

RN 396718-59-5 HCAPLUS

CN Carbamic acid, [2-[[9-[N-ethyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranuronamidosyl]-9H-purin-6-yl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

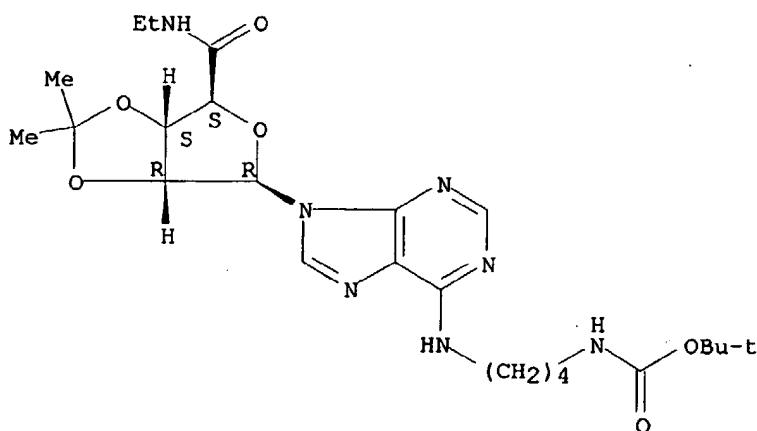
Absolute stereochemistry.



RN 396718-60-8 HCAPLUS

CN Carbamic acid, [4-[[9-[N-ethyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranuronamidosyl]-9H-purin-6-yl]amino]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

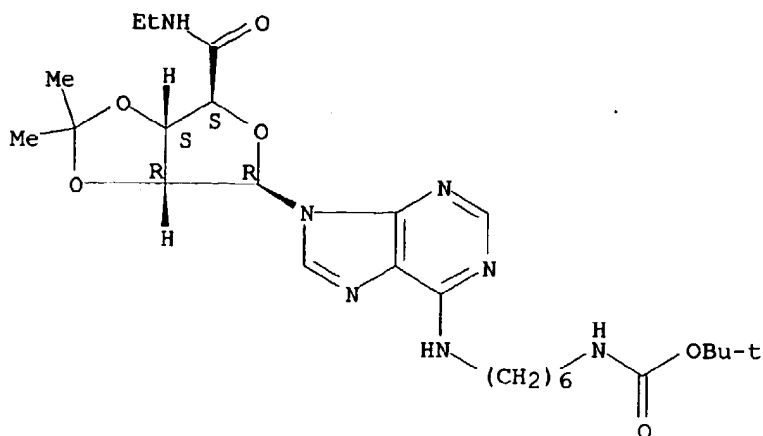
Absolute stereochemistry.



RN 396718-61-9 HCAPLUS

CN Carbamic acid, [6-[[9-[N-ethyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranuronamidosyl]-9H-purin-6-yl]amino]hexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

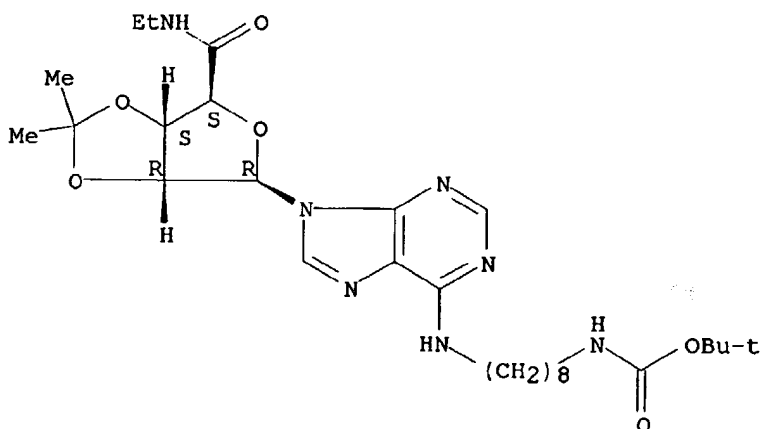
Absolute stereochemistry.



RN 396718-62-0 HCAPLUS

CN Carbamic acid, [8-[[9-[N-ethyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranuronamidosyl]-9H-purin-6-yl]amino]octyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

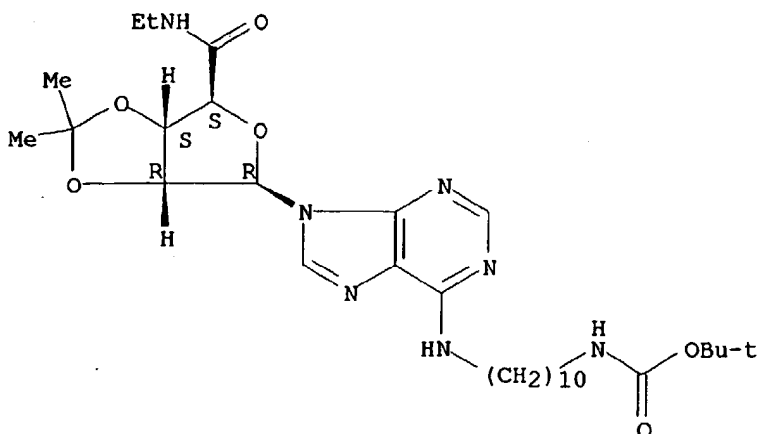
Absolute stereochemistry.



RN 396718-63-1 HCAPLUS

CN Carbamic acid, [10-[[9-[N-ethyl-2,3-O-(1-methylethylidene)-.beta.-D-ribofuranuronamidosyl]-9H-purin-6-yl]amino]decyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

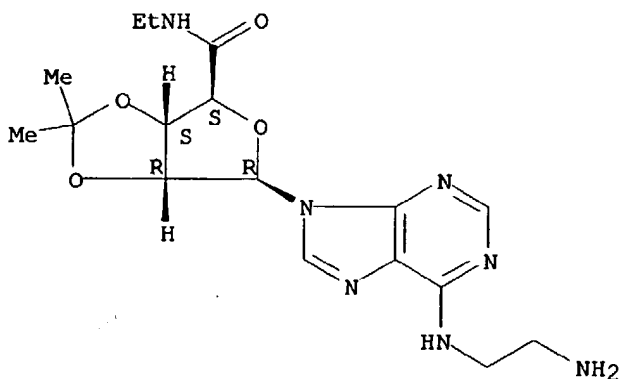
Absolute stereochemistry.



RN 396718-64-2 HCAPLUS

CN .beta.-D-Ribofuranuronamide, 1-[6-[(2-aminoethyl)amino]-9H-purin-9-yl]-1-deoxy-N-ethyl-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

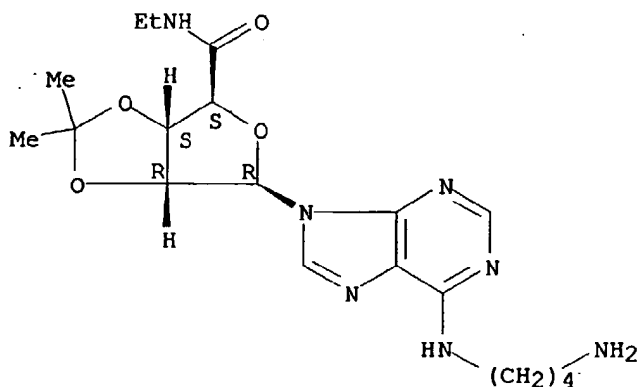
Absolute stereochemistry.



RN 396718-65-3 HCAPLUS

CN .beta.-D-Ribofuranuronamide, 1-[6-[(4-aminobutyl)amino]-9H-purin-9-yl]-1-deoxy-N-ethyl-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

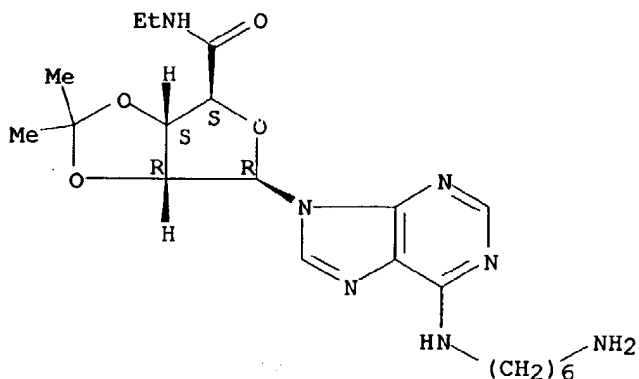
Absolute stereochemistry.



RN 396718-67-5 HCAPLUS

CN .beta.-D-Ribofuranuronamide, 1-[6-[(6-aminohexyl)amino]-9H-purin-9-yl]-1-deoxy-N-ethyl-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 396718-69-7 HCAPLUS

CN .beta.-D-Ribofuranuronamide, 1-[6-[(8-amino-octyl)amino]-9H-purin-9-yl]-1-deoxy-N-ethyl-2,3-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.